

10509228

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PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 17:26:55 ON 12 OCT 2006
FILE 'REGISTRY' ENTERED AT 17:26:55 ON 12 OCT 2006
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COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.28	5.49

=> file reg

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.72	5.93

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STRUCTURE FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8
DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> set postings on
SET COMMAND COMPLETED

=> s heterocyclic and aldehyde
2 HETEROCYCLIC
296422 ALDEHYDE
24 ALDEHYDES
296422 ALDEHYDE
(ALDEHYDE OR ALDEHYDES)
L4 0 HETEROCYCLIC AND ALDEHYDE

Updated Search

10509228

=> s aldehyde?

L5 296422 ALDEHYDE?

=> s heterocyclic

L6 2 HETEROCYCLIC

=> s l6 and l5

L7 0 L6 AND L5

=> s hydroxymethyl

L8 275636 HYDROXYMETHYL

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

24.68

30.61

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16

FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006

SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE

L5 296422 S ALDEHYDE?

L6 2 S HETEROCYCLIC

L7 0 S L6 AND L5

L8 275636 S HYDROXYMETHYL

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FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

=> s l5/prep
751488 L5
3539700 PREP/RL
L9 144752 L5/PREP
(L5 (L) PREP/RL)

=>

=> s l8/rct
458850 L8
2897022 RCT/RL
L10 100866 L8/RCT
(L8 (L) RCT/RL)

=> s l10 (1) l9
L11 982 L10 (L) L9

=> file hcaplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	15.18	45.79

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006
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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s hypohalogenous? () salt?
53 HYPOHALOGENOUS?
1175891 SALT?
L12 1 HYPOHALOGENOUS? (W) SALT?

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006
L1 STRUCTURE UPLOADED

Updated Search

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L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?

=> s l12 l11
MISSING OPERATOR L12 L11
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l12 () l11
PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
FIELD CODE - 'AND' OPERATOR ASSUMED 'L12 (W) L11'
L13 0 L12 (W) L11

=> s l12 and l11
L14 0 L12 AND L11

=> s halogen?
L15 166106 HALOGEN?

=> s l15 () l11
PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
FIELD CODE - 'AND' OPERATOR ASSUMED 'L15 (W) L11'
L16 28 L15 (W) L11

=> s l12 (l) l11
L17 0 L12 (L) L11

=> s l12 and l11
L18 0 L12 AND L11

=> s l15 and l11
L19 28 L15 AND L11

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.59	53.38

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006
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STRUCTURE FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8
DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> set postings on
SET COMMAND COMPLETED

=> s tetramethyl and piperidine
383162 TETRAMETHYL
2 TETRAMETHYLS
383162 TETRAMETHYL
(TETRAMETHYL OR TETRAMETHYLS)
394986 PIPERIDINE
L20 6024 TETRAMETHYL AND PIPERIDINE

=> s l20 and oxyl
7516 OXYL
L21 92 L20 AND OXYL

=> s "2,2,6,6-tetramethyl" and piperidine and "1-oxyl"
32058 "2,2,6,6"
383162 "TETRAMETHYL"
2 "TETRAMETHYLS"
383162 "TETRAMETHYL"
("TETRAMETHYL" OR "TETRAMETHYLS")
30406 "2,2,6,6-TETRAMETHYL"
("2,2,6,6" (W) "TETRAMETHYL")
394986 PIPERIDINE
19346742 "1"
7516 "OXYL"
295 "1-OXYL"
("1" (W) "OXYL")
L22 69 "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

=> d l22, all

L22 ANSWER 1 OF 69 REGISTRY COPYRIGHT 2006 ACS on STN
RN 347362-24-7 REGISTRY
ED Entered STN: 23 Jul 2001
CN 1-Piperidinyloxy, 4-[(9-anthracenylcarbonyl)oxy]-2,2,6,6-tetramethyl-
(9CI) (CA INDEX NAME)
OTHER NAMES:
CN 4-(9-Anthroyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl

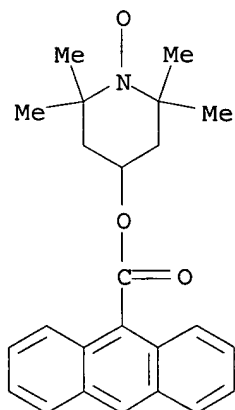
Updated Search

10509228

MF C24 H26 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation);
PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
(Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N	NC5	6	C5N	46.156.1	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2508.17.56	1



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 136:199849 CA
TI Anthracene Derivatives and the Corresponding Dimers with TEMPO Radicals
AU Nakatsuji, Shin'ichi; Ojima, Takeo; Akutsu, Hiroki; Yamada, Junichi
CS Department of Material Science Faculty of Science, Himeji Institute of
Technology, Kamigori, Hyogo, 678-1297, Japan
SO Journal of Organic Chemistry (2002), 67(3), 916-921
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 74, 77
AB Anthracene derivs. with several TEMPO radicals 9-C14H9-X-TEMPO where X is
a linker from the 9 position of anthracene to the 4 position of TEMPO [X =
CONH, CONMe, CO2, CH2NH (2, 3, 4, and 10, resp.)] were prepared, and each
photodimerization reaction was investigated. Although the

Updated Search

photodimerization was unsuccessful in obtaining the dimers of anthracenes 2 and 3, which could be alternatively prepared in a stepwise manner, the photodimers (all photodimers trans in this abstract) of anthracenes 4 and 10 were available by the direct photoreaction. The dissociation reaction of the dimers proceeded well by heating them in solution to give the corresponding monomers in each case, and thus the reversible system could be constructed in the latter two systems. While no large difference was observed in their magnetic behaviors between the monomer/dimer pair of monomer 4 and dimer 8, an intriguing difference was found in the magnetic behaviors for the pair of monomer 10 and dimer 11 from ferromagnetic interactions in 10 to the variable magnetic interactions in 11 depending on the solvent mols. incorporated in the crystals.

- ST anthracene TEMPO deriv photodimerization magnetic property
- IT Hydrogen bond
(ferromagnetic coupling through hydrogen bonds; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Dimerization
(photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Antiferromagnetic exchange
Configuration
Curie-Weiss law
ESR (electron spin resonance)
Exchange interaction
Ferromagnetic exchange
Magnetic susceptibility
Solvates
Zero field splitting
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Nitroxides
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Clathrates
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT Ring opening
(thermal; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 14691-88-4, 4-Amino-TEMPO
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation and reductive amination; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 723-62-6, 9-Anthracenecarboxylic acid 108654-32-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 42585-33-1P, 4-(Methylamino)-TEMPO
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amidation; preparation and reversible photodimerization of anthracene TEMPO

- derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 363148-79-2P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (attempted direct photodimerization, crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-23-6P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (attempted direct photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-91-0P 295797-93-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-89-6P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (direct photodimerization, crystallog.; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-24-7P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (direct photodimerization; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-92-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 2226-96-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 347362-25-8P 401796-52-9P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation from 9-anthracenecarboxylic acid photodimer; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 150809-84-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (reduction; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 642-31-9, 9-Anthraldehyde 2896-70-0, 4-Oxo-TEMPO
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reductive amination; preparation and reversible photodimerization of anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)
- IT 295797-90-9P 347362-26-9P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (thermal cycloreversion; preparation and reversible photodimerization of

anthracene TEMPO derivs., and crystallog. and magnetic properties of the monomers and dimers)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (2) Akutsu, H; Synth Met 2001, V120, P871 CAPLUS
- (3) Bouas-Laurent, H; Chem Soc Rev 2000, V29, P43 CAPLUS
- (4) Cowan, D; J Am Chem Soc 1972, V94, P6779 CAPLUS
- (5) Gu, Z; J Phys Chem 1996, V100, P18290
- (6) Hamachi, K; Bull Chem Soc Jpn 1998, V71, P2937 CAPLUS
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- (10) Matsuda, K; Chem Lett 2001, P436 CAPLUS
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REFERENCE 2

AN 136:47590 CA
 TI Investigation of the anthracene-nitroxide hybrid molecule as a probe for hydroxyl radicals
 AU Yang, Xiao-Feng; Guo, Xiang-Qun
 CS Department of Chemistry and the Key Laboratory of Analytical Sciences of MOE, Xiamen University, Xiamen, 361005, Peop. Rep. China
 SO Analyst (Cambridge, United Kingdom) (2001), 126(10), 1800-1804
 CODEN: ANALAO; ISSN: 0003-2654
 PB Royal Society of Chemistry
 DT Journal
 LA English
 CC 79-3 (Inorganic Analytical Chemistry)
 AB A new method for the determination of hydroxyl radicals is proposed. The method is based on the use of a hybrid mol. consisting of a fluorescent chromophore, anthracene, and a nitroxide radical. In the hybrid mol., the nitroxide quenches the fluorescence of anthracene strongly. The reaction of hydroxyl radicals with DMSO generates quant. Me radicals, which then combine with the nitroxide moiety of the hybrid mols. to result in an increase in the fluorescence intensity. The fluorescence increase is

proportional to the concentration of hydroxyl radicals. The proposed method is capable of detecting hydroxyl radicals generated in the Fenton system. It is a simple and sensitive technique for the determination of hydroxyl radicals.

ST anthracene nitroxide hybrid mol hydroxyl radical

IT Absorption spectra

Chromophores

Fenton reaction

Fluorescence

Fluorometry

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 3352-57-6, Hydroxyl, analysis 380202-05-1

RL: ANT (Analyte); ANST (Analytical study)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 347362-24-7P, 4-(9-Anthroyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl

RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST (Analytical study); PREP (Preparation); USES (Uses)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 723-62-6, 9-Anthracenecarboxylic acid 2226-96-2,

4-Hydroxy-2,2,6,6-tetramethylpiperidinyloxy

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 16331-52-5P, 9-Anthracenecarboxylic acid chloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydroxyl radical determination by fluorometry using anthracene linked to

TEMPO

as fluorescent chromophore)

IT 67-68-5, DMSO, uses

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(hydroxyl trapping agent; hydroxyl radical determination by fluorometry

using

anthracene linked to TEMPO as fluorescent chromophore)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (33) Ste-Marie, L; Anal Biochem 1996, V241, P67 CAPLUS
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- (35) Yang, C; J Chromatogr B 1997, V693, P257 CAPLUS
- (36) Zweier, J; Proc Natl Acad Sci 1987, V84, P1404 CAPLUS

REFERENCE 3

- AN 135:272668 CA
- TI Magnetic properties of anthracene derivatives and the corresponding photo-dimers with stable radical substituents
- AU Ojima, T.; Akutsu, H.; Yamada, J.-i.; Nakatsuji, S.
- CS Faculty of Science, Department of Material Science, Himeji Institute of Technology, Kamigori, Hyogo, 678-1297, Japan
- SO Polyhedron (2001), 20(11-14), 1335-1338
CODEN: PLYHDE; ISSN: 0277-5387
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- CC 22-13 (Physical Organic Chemistry)
Section cross-reference(s): 75, 77
- AB Several anthracene derivs. with stable radical substituents have been prepared and their magnetic properties have been investigated together with those of some of the dimers available by photo-dimerization reaction. While weak magnetic interactions with Curie-Weiss behavior have been observed in most derivs. prepared, antiferromagnetic behavior being based on an S-T model has been found in the spins of TEMPO-substituted N-methylcarboxyamidoanthracene derivative 1c. The magnetic property of Mn(hfac)₂ complex derived from 4-amino-TEMPO-substituted 9-methylanthracene (1d) is also described.
- ST TEMPO substituted magnetic property crystallog
- IT Antiferromagnetism
Crystal structure
Curie-Weiss law
Magnetic properties
Magnetic susceptibility
Molecular structure
(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)
- IT Nitroxides
RL: PRP (Properties)
(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)
- IT 178170-34-8 295797-89-6 295797-90-9 347362-23-6 347362-24-7
347362-25-8 347362-26-9 363148-79-2 363158-33-2
RL: PRP (Properties)

(magnetic properties of anthracene derivs. and corresponding photodimers with stable nitroxide radical substituents)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Caneschi, A; Inorg Chem 1988, V27, P2027 CAPLUS
- (2) Dickman, M; Inorg Chem 1986, V25, P2595 CAPLUS
- (3) Gutlich, P; Angew Chem Int Ed 1994, V33, P2024
- (4) Hamachi, K; Bull Chem Soc 1998, V71, P2937 CAPLUS
- (5) Matsuda, K; Chem Lett 2000, P16 CAPLUS
- (6) Matsuda, K; J Am Chem Soc 2000, V122, P7195 CAPLUS
- (7) Matsuda, K; J Am Chem Soc 2000, V122, P8309 CAPLUS
- (8) Matsuda, K; Tetrahedron Lett 2000, V41, P2577 CAPLUS
- (9) Nagai, K; Solid State Commun 1997, V102, P809 CAPLUS
- (10) Nakatsuji, S; J Chem Soc, Perkin Trans 2 2000, P1969 CAPLUS
- (11) Nakatsuji, S; Mol Cryst Liq Cryst 1996, V279, P73 CAPLUS
- (12) Nakatsuji, S; Mol Cryst Liq Cryst 2000, V348, P1 CAPLUS
- (13) Nakatsuji, S; Mol Cryst Liq Cryst in press 2001
- (14) Nakatsuji, S; Mol Cryst Liq Cryst in press 2001
- (15) Ojima, T; Chem Lett 2000, P918 CAPLUS
- (16) Sato, O; Science 1996, V272, P704 CAPLUS
- (17) Takeuchi, S; Mol Cryst Liq Cryst 2000, V345, P167 CAPLUS
- (18) Verdaguer, M; Science 1996, V272, P698 CAPLUS

REFERENCE 4

- AN 135:84149 CA
- TI Preparation and properties of photofunctional systems with nitroxide radicals
- AU Nakatsuji, Shin'ichi; Takeuchi, Soichi; Ojima, Takeo; Ogawa, Yuya; Akutsu, Hiroki; Yamada, Jun-Ichi
- CS Department of Material Science, Faculty of Science, Himeji Institute of Technology, Kamigori, 678-1297, Japan
- SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2001), 356, 23-32
CODEN: MCLCE9; ISSN: 1058-725X
- PB Gordon & Breach Science Publishers
- DT Journal
- LA English
- CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 77
- AB Series of TEMPO-substituted norbornadiene, spiropyran and anthracene derivs. have been prepared: their light-induced structural change to the corresponding quadricyclanes, merocyanines or anthracene-dimers and the reverse reactions to the starting materials have been studied. The antiferromagnetic or ferromagnetic behavior observed in norbornadienes/anthracenes was found to be preserved in the corresponding quadricyclanes/anthracene-dimers in spite of the difference of their Weiss temps., whereas switching of the intermol. magnetic interactions was observed in spiropyran/merocyanine systems.
- ST photofunctional organomagnēt nitroxide radical substituted mol photoreaction; norbornadiene piperidyloxy substituted org photoreactive mol magnetic property; spiropyran piperidyloxy substituted org photoreactive mol magnetic property; anthracene piperidyloxy substituted org photoreactive mol magnetic property
- IT Ring opening
(photochem.; photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnēt system)
- IT Dimerization

- (photodimerization; photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT Antiferromagnetic materials
Curie-Weiss law
Ferromagnetic materials
Magnetic properties
Magnetic susceptibility
Photolysis
(photofunctional organomagnets including methylpiperidyloxy-substituted norbornadiene- and spiropyran- and anthracene derivs.)
- IT Isomerization
(valence, photochem.; photoinduced reversible reactions and properties of methylpiperidyloxy-substituted norbornadiene derivative photofunctional organomagnets)
- IT 347362-25-8 347362-26-9
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT 347362-21-4 347362-22-5 347362-23-6 347362-24-7
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted anthracene derivative/ photodimer photofunctional organomagnet system)
- IT 307307-48-8P 307307-49-9P 307307-50-2P
RL: FMU (Formation, unclassified); PNU (Preparation, unclassified); PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted norbornadiene derivative/ qudricyclane photofunctional organomagnet system)
- IT 307307-45-5P 307307-46-6P 307307-47-7P
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); PROC (Process)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted norbornadiene derivative/ qudricyclane photofunctional organomagnet system)
- IT 347362-29-2 347362-30-5
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnet system)
- IT 347362-27-0 347362-28-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photoinduced reactions and magnetic properties of methylpiperidyloxy-substituted spiropyran derivative/ merocyanine photofunctional organomagnet system)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Cowan, D; J Am Chem Soc 1972, V94, P6779 CAPLUS
- (2) Cristol, S; J Am Chem Soc 1958, V80, P1950 CAPLUS
- (3) Guglielmetti, R; Photochromism: Molecules and Systems 1990
- (4) Gutlich, P; Angew, Chem Int Ed 1994, V33, P2024
- (5) Hamachi, K; Bull Chem Soc 1998, V71, P2937 CAPLUS

10509228

- (6) Hassner, A; Tetrahedron Lett 1978, V46, P4475
- (7) Hautala, R; Solar Energy Chemical Conversion and Storage 1979
- (8) Matsuda, K; the Annual Meeting of Chemical Society of Japan held in Yokohama 1999, 3G2 16, P404
- (9) Nagai, K; Solid State Commun 1997, V102, P809 CAPLUS
- (10) Nakatsuji, S; New J Chem 1998, P275 CAPLUS
- (11) Namba, K; Bull Chem Soc 1975, V48, P1323 CAPLUS
- (12) Natatsuji, S; J Mater Chem 1997, V7, P2161
- (13) Sato, O; Science 1996, V272, P704 CAPLUS
- (14) Schonberg, A; Preparative Organic Photochemistry 1968
- (15) Verdaguer, M; Science 1996, V272, P698 CAPLUS

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
L14 0 S L12 AND L11
L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
44.62	98.00

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.71	-0.71

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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

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=> s l21
L23 7022 L21

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L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006
SET POSTINGS ON
L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006
L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006
L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
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L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

Updated Search

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FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006
SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006
L23 7022 S L21

=> s l23 and l11
L24 1 L23 AND L11

=> d l24, ibib abs hitstr, 1

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:213306 HCAPLUS

DOCUMENT NUMBER: 140:253453

TITLE: Process for the preparation of 1,3-dihydro-6-methylfuro(3,4-c)pyridin-7-ol derivatives, in particular cicletanine hydrochloride, by protection, oxidation, addition of a nucleophile, and one pot deprotection/cyclodehydration

INVENTOR(S): Gore, Vinayak G.; Ghadge, Manoj M.; Gupta, Ashwini Kumar K.

PATENT ASSIGNEE(S): Generics (UK) Limited, UK

SOURCE: Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

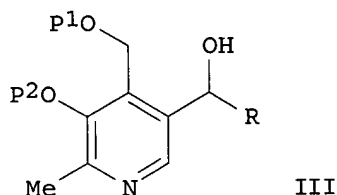
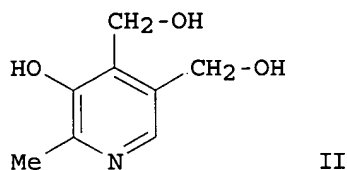
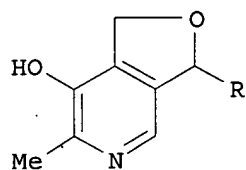
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398316	A2	20040317	EP 2003-255795	20030916
EP 1398316	A3	20040414		
EP 1398316	B1	20060614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 329918	E	20060715	AT 2003-255795	20030916
PRIORITY APPLN. INFO.:			GB 2002-21494	A 20020916
OTHER SOURCE(S):		CASREACT 140:253453; MARPAT 140:253453		
GI				



AB The invention is directed to the preparation of 1,3-dihydro-6-methylfuro(3,4-c)pyridin-7-ols I or salt by selective protection of pyridoxine II or salt, oxidation of the 3,4-protected pyridoxine with aqueous NaClO in the presence of catalytic amount of TEMPO, addition of a nucleophile, especially a Grignard reagent,

to the 3,4-protected pyridoxal, and one pot deprotection/cyclodehydration of III [R = substituted al(en/yn)yl, alkyl/alkenyl/alkynyl/aryl, arylalk(en/yn)yl which may include one or more N, O, or S; P1, P2 = independently protecting groups or together form one protecting group]. The invention is directed in particular to preparation of the well-known antihypertensive agent cicletanine hydrochloride (I•HCl, where R = 4-chlorophenyl). The advantages include environmentally friendly starting materials, simple process, and therefore an easy industrial scale-up. For example, cicletanine hydrochloride was prepared protection of pyridoxine hydrochloride with acetone/HCl, oxidation of the pyridinylmethyl alc. with NaClO in the presence of TEMPO/NaHCO₃/DCM, addition of the 4-chlorophenylmagnesium bromide generated in situ from Mg and 4-bromochlorobenzene in THF at reflux, followed by one pot deprotection/cyclodehydration with concentrated HCl at reflux.

IT 6560-65-2P

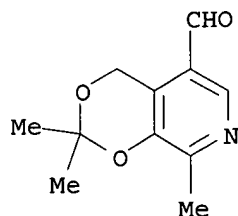
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(aldehyde intermediate; process for preparation of cicletanine hydrochloride and its derivs. by protection, oxidation, addition of a nucleophile, and one pot deprotection/cyclodehydration)

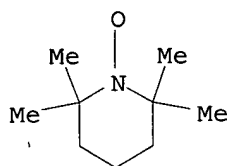
RN 6560-65-2 HCAPLUS

CN 4H-1,3-Dioxino[4,5-c]pyridine-5-carboxaldehyde, 2,2,8-trimethyl- (9CI)
(CA INDEX NAME)

10509228



IT 2564-83-2, 2,2,6,6-Tetramethyl-1-piperidinyloxy
RL: CAT (Catalyst use); USES (Uses)
(catalyst; process for preparation of cicletanine hydrochloride and its
derivs. by protection, oxidation, addition of a nucleophile, and one pot
deprotection/cyclodehydration)
RN 2564-83-2 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



=> file caold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
50.65	148.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-1.46

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006

SET POSTINGS ON
L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
L14 0 S L12 AND L11
L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON
L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

=> s l11 and l22 and l8
TOO MANY TERMS FOR FILE CROSSOVER IN L8
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> s l11 and l22
TOO MANY TERMS FOR FILE CROSSOVER IN L8
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> s l11 and l22
TOO MANY TERMS FOR FILE CROSSOVER IN L8
There are limits on the size of an answer set being crossed over from

Updated Search

10509228

one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s l22

L25 59 L22

=> s l11

TOO MANY TERMS FOR FILE CROSSOVER IN L8

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=> s l11

TOO MANY TERMS FOR FILE CROSSOVER IN L8

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.20	150.85

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.46

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DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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SET COMMAND COMPLETED

=> s "1-oxyl-4-yl" and tetramethyl and piperidine

19346742 "1"

7516 "OXYL"

17443241 "4"

Updated Search

10509228

15372835 "YL"
210 "YLS"
15372835 "YL"
("YL" OR "YLS")
5 "1-OXYL-4-YL"
("1" (W) "OXYL" (W) "4" (W) "YL")
383162 TETRAMETHYL
2 TETRAMETHYLS
383162 TETRAMETHYL
(TETRAMETHYL OR TETRAMETHYLS)
394986 PIPERIDINE
L26 1 "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE

=> d 126

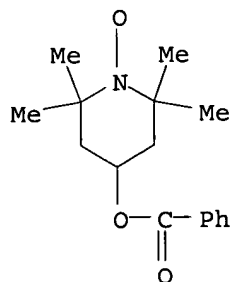
L26 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 3225-26-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA
INDEX NAME)

OTHER CA INDEX NAMES:

CN Piperidinooxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)
CN Piperidinooxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester)
(8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxyl
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidinyl-1-oxyl benzoate
CN Tempol benzoate
MF C16 H22 N O3
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CSChem, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

251 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006

SET POSTINGS ON
L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
L14 0 S L12 AND L11
L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON
L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006

SET POSTINGS ON
L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE

=> s "2,2,6,6-tetramethyl" and piperidine and "1-oxyl-4-yl"

Updated Search

10509228

32058 "2,2,6,6"
383162 "TETRAMETHYL"
2 "TETRAMETHYLS"
383162 "TETRAMETHYL"
("TETRAMETHYL" OR "TETRAMETHYLS")
30406 "2,2,6,6-TETRAMETHYL"
("2,2,6,6" (W) "TETRAMETHYL")
394986 PIPERIDINE
19346742 "1"
7516 "OXYL"
17443241 "4"
15372835 "YL"
210 "YLS"
15372835 "YL"
("YL" OR "YLS")
5 "1-OXYL-4-YL"
("1" (W) "OXYL" (W) "4" (W) "YL")
L27 1 "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

=>. d 127

L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 3225-26-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA
INDEX NAME)

OTHER CA INDEX NAMES:

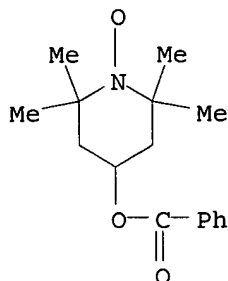
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester)
(8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxy
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidinyl-1-oxyl benzoate
CN Tempol benzoate
MF C16 H22 N O3
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CSCHEM, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

Updated Search

10509228



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

251 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006
SET POSTINGS ON

L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
L14 0 S L12 AND L11
L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

Updated Search

10509228

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006
L23 7022 S L21
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006
L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006
SET POSTINGS ON
L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE
L27 1 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
67.00	217.85

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.46

CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 17:50:43 ON 12 OCT 2006
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FILE COVERS 1907 - 12 Oct 2006 VOL 145 ISS 16
FILE LAST UPDATED: 11 Oct 2006 (20061011/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l27
L28 251 L27

=> d his

(FILE 'HOME' ENTERED AT 17:09:19 ON 12 OCT 2006)

FILE 'REGISTRY' ENTERED AT 17:09:29 ON 12 OCT 2006
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 6 S L2

FILE 'REGISTRY' ENTERED AT 17:27:25 ON 12 OCT 2006
SET POSTINGS ON

Updated Search

10509228

L4 0 S HETEROCYCLIC AND ALDEHYDE
L5 296422 S ALDEHYDE?
L6 2 S HETEROCYCLIC
L7 0 S L6 AND L5
L8 275636 S HYDROXYMETHYL

FILE 'HCAPLUS' ENTERED AT 17:28:42 ON 12 OCT 2006

L9 144752 S L5/PREP
L10 100866 S L8/RCT
L11 982 S L10 (L) L9

FILE 'HCAPLUS' ENTERED AT 17:32:05 ON 12 OCT 2006

L12 1 S HYPOHALOGENOUS? () SALT?
L13 0 S L12 () L11
L14 0 S L12 AND L11
L15 166106 S HALOGEN?
L16 28 S L15 () L11
L17 0 S L12 (L) L11
L18 0 S L12 AND L11
L19 28 S L15 AND L11

FILE 'REGISTRY' ENTERED AT 17:33:49 ON 12 OCT 2006

SET POSTINGS ON

L20 6024 S TETRAMETHYL AND PIPERIDINE
L21 92 S L20 AND OXYL
L22 69 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL"

FILE 'HCAPLUS' ENTERED AT 17:35:30 ON 12 OCT 2006

L23 7022 S L21
L24 1 S L23 AND L11

FILE 'CAOLD' ENTERED AT 17:46:23 ON 12 OCT 2006

L25 59 S L22

FILE 'REGISTRY' ENTERED AT 17:49:06 ON 12 OCT 2006

SET POSTINGS ON

L26 1 S "1-OXYL-4-YL" AND TETRAMETHYL AND PIPERIDINE
L27 1 S "2,2,6,6-TETRAMETHYL" AND PIPERIDINE AND "1-OXYL-4-YL"

FILE 'HCAPLUS' ENTERED AT 17:50:43 ON 12 OCT 2006

L28 251 S L27

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.53	220.38

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.46

CA SUBSCRIBER PRICE

FILE 'CAOLD' ENTERED AT 17:50:57 ON 12 OCT 2006
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

Updated Search

10509228

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l27 and l25

2 L27

L29 2 L27 AND L25

=> d l29, all, 1-2

L29 ANSWER 1 OF 2 CAOLD COPYRIGHT 2006 ACS on STN

AN CA65:10559e CAOLD

TI synthesis of heterocyclic analogs of hydroxylamine

AU Rozantsev, E. G.; Golubev, V. A.

IT 768-66-1 850-43-1 3225-26-1 3637-10-3 3637-11-4

4972-13-8 7031-85-8 7031-86-9 7031-87-0 7031-88-1 7031-89-2

7031-90-5 7031-92-7 7031-93-8 7031-94-9 7031-95-0 7031-96-1

7032-00-0 7032-01-1 7166-32-7 10439-48-2 16203-28-4

L29 ANSWER 2 OF 2 CAOLD COPYRIGHT 2006 ACS on STN

AN CA62:14621b CAOLD

TI free radicals in iminoxyl series in the group of hydrogenated pyridine

AU Rozantsev, E. G.; Golubev, V. A.; Neiman, M. B.

TI preparation of N-tert-butyl-4-piperidone

AU Robinson, John Barry; Thomas, J.

IT 1462-98-2 1462-99-3 1463-00-9 1465-76-5 1742-82-1 1796-15-2

1796-16-3 1796-17-4 1796-18-5 1796-19-6 1796-20-9 2013-75-4

2234-55-1 3225-24-9 3225-25-0 3225-26-1 3225-27-2

3264-93-5

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.78

222.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-1.46

FILE 'REGISTRY' ENTERED AT 17:51:21 ON 12 OCT 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

Updated Search

10509228

DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 3225-26-1/RN

L30 1 3225-26-1/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L30 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L30 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 3225-26-1 REGISTRY
CN 1-Piperidinyloxy, 4-(benzoyloxy)-2,2,6,6-tetramethyl- (9CI) (CA INDEX
NAME)

OTHER CA INDEX NAMES:

CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (7CI)
CN Piperidinoxy, 4-hydroxy-2,2,6,6-tetramethyl-, benzoate (ester) (8CI)

OTHER NAMES:

CN 1-Oxyl-2,2,6,6-tetramethylpiperidin-4-yl benzoate
CN 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine
CN 2,2,6,6-Tetramethyl-4-(benzoyloxy)piperidine-1-oxyl
CN 2,2,6,6-Tetramethyl-4-benzoatepiperidine-1-oxy
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine N-oxide
CN 2,2,6,6-Tetramethyl-4-benzoyloxypiperidine-1-oxy radical
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidin-1-oxyl benzoate
CN 2,2,6,6-Tetramethyl-4-hydroxypiperidine-1-oxyl benzoate
CN 2,2,6,6-Tetramethylpiperidin-1-oxyl-4-yl benzoate
CN 4-(Benzoyloxy)-2,2,6,6-tetramethyl-1-piperidinyloxy
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidin-1-yloxy
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-1-oxyl
CN 4-(Benzoyloxy)-2,2,6,6-tetramethylpiperidine-N-oxyl
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl benzoate
CN 4-Hydroxy-2,2,6,6-tetramethylpiperidiny-1-oxyl benzoate
CN Tempol benzoate

MF C16 H22 N O3

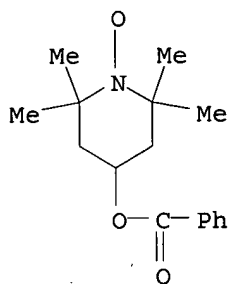
CI COM

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CSChem, DDFU, DRUGU, TOXCENTER, USPAT2, USPATFULL

Updated Search

10509228

(*File contains numerically searchable property data)
DT.CA Caplus document type: Conference; Journal; Patent
RL.P Roles from patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

251 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
251 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

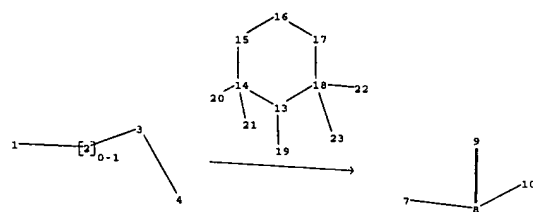
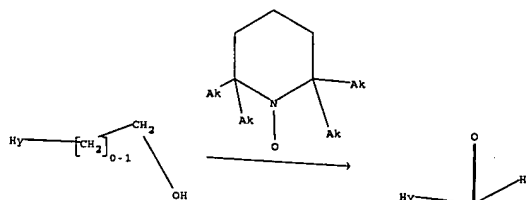
=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=>

=>

Updated Search



chain nodes :

1 2 3 4 7 8 9 10 19 20 21 22 23

ring nodes :

13 14 15 16 17 18

chain bonds :

1-2 2-3 3-4 7-8 8-9 8-10 13-19 14-20 14-21 18-22 18-23

ring bonds :

13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-2 7-8 8-9 13-14 13-18 13-19 14-15 14-20 14-21 15-16 16-17 17-18 18-22 18-23

exact bonds :

2-3 3-4 8-10

isolated ring systems :

containing 13 :

Match level :

1:Atom 2:CLASS3:CLASS4:CLASS7:Atom 8:CLASS9:CLASS10:CLASS13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS

fragments assigned reactant role:

containing 1

fragments assigned reagent role:

containing 13

fragments assigned product role:

10509228

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal612bxr

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	4	MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS	5	MAY 11	KOREAPAT updates resume
NEWS	6	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS	7	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPATFULL/USPAT2
NEWS	8	MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS	9	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS	10	JUN 26	TULSA/TULSA2 reloaded and enhanced with new search and and display fields
NEWS	11	JUN 28	Price changes in full-text patent databases EPFULL and PCTFULL
NEWS	12	JUL 11	CHEMSAFE reloaded and enhanced
NEWS	13	JUL 14	FSTA enhanced with Japanese patents
NEWS	14	JUL 19	Coverage of Research Disclosure reinstated in DWPI
NEWS	15	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS	16	AUG 28	ADISCTI Reloaded and Enhanced
NEWS	17	AUG 30	CA(SM)/CAPLUS(SM) Austrian patent law changes
NEWS	18	SEP 11	CA/CAPLUS enhanced with more pre-1907 records
NEWS	19	SEP 21	CA/CAPLUS fields enhanced with simultaneous left and right truncation
NEWS	20	SEP 25	CA(SM)/CAPLUS(SM) display of CA Lexicon enhanced
NEWS	21	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS	22	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS	23	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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Updated Search

10509228

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

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FILE CONTENT:1840 - 8 Oct 2006 VOL 145 ISS 15

New CAS Information Use Policies, enter HELP USAGETERMS for details.

* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\oioi.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 19:54:15 FILE 'CASREACT'

SCREENING COMPLETE - 6029 REACTIONS TO VERIFY FROM

147 DOCUMENTS

82.9% DONE 5000 VERIFIED 12 HIT RXNS

3 DOCS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 115946 TO 125214

PROJECTED ANSWERS: 3 TO 213

L2 3 SEA SSS SAM L1 (12 REACTIONS)

Updated Search

10509228

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 109.70 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 19:54:20 FILE 'CASREACT'

SCREENING COMPLETE - 119561 REACTIONS TO VERIFY FROM 3061 DOCUMENTS

100.0% DONE 119561 VERIFIED 131 HIT RXNS 38 DOCS

SEARCH TIME: 00.00.05

L3 38 SEA SSS FUL L1 (131 REACTIONS)

=> s l3 and shiomi, y?/au

18 SHIOMI, Y?/AU

L4 0 L3 AND SHIOMI, Y?/AU

=> s l3 and uno, o?/au

9 UNO, O?/AU

L5 0 L3 AND UNO, O?/AU

=> s l3 and ohta, a?/au

89 OHTA, A?/AU

L6 0 L3 AND OHTA, A?/AU

=> s l3 and sunakami, t?/au

0 SUNAKAMI, T?/AU

L7 0 L3 AND SUNAKAMI, T?/AU

=> d l3, ibib abs hit, 1-38

L3 ANSWER 1 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 145:64877 CASREACT

TITLE: Conversion of 2,5-(hydroxymethyl)furaldehyde to industrial derivatives, purification of the derivatives, and industrial uses therefor

INVENTOR(S): Sanborn, Alexandra, J.; Bloom, Paul, D.

PATENT ASSIGNEE(S): Archer-Daniels-Midland Company, USA

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006063287	A2	20060615	WO 2005-US44721	20051209
WO 2006063287	A3	20060914		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,			

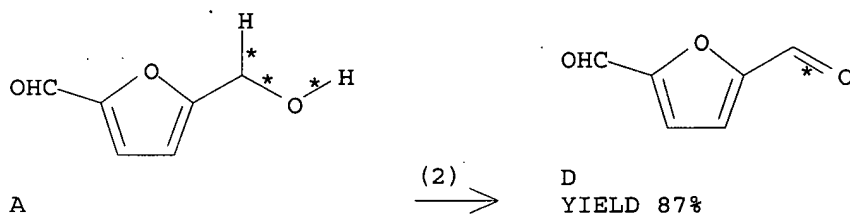
Updated Search

10509228

KG, KZ, MD, RU, TJ, TM			
US 2006128843	A1	20060615	US 2005-70063 20050302
US 2006128977	A1	20060615	US 2005-273947 20051115
US 2006128844	A1	20060615	US 2005-274554 20051115
US 2006142599	A1	20060629	US 2005-298014 20051209
PRIORITY APPLN. INFO.:			US 2004-635406P 20041210
			US 2005-70063 20050302

AB A method of preparing 2,5-bis(hydroxymethyl)tetrahydrofuran comprises heating a reaction mixture comprising 2,5-(hydroxymethyl)furaldehyde, an organic solvent, and a catalyst system comprising nickel and zirconium at a temperature, for a time, and at a pressure sufficient to promote reduction of the 2,5-(hydroxymethyl)furaldehyde to 2,5-bis(hydroxymethyl)tetrahydrofuran to produce a product mixture comprising 2,5-bis(hydroxymethyl)tetrahydrofuran. 2,5-Furandialdehyde is also prepared 2,5-Bis(hydroxymethyl)tetrahydrofuran is useful in coatings.

RX(2) OF 2 A ==> D



RX(2) RCT A 67-47-0
 RGT E 2564-83-2 Me4-piperidoxyl, F 3240-34-4 PhI(OAc)2
 PRO D 823-82-5
 SOL 108-10-1 i-BuCOMe
 CON 1.5 hours, room temperature
 NTE optimization study

L3 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 144:232853 CASREACT
 TITLE: A process for the preparation of rosuvastatin involving a TEMPO-mediated oxidation step
 INVENTOR(S): Niddam-Hildesheim, Valerie; Chen, Kobi
 PATENT ASSIGNEE(S): Teva Pharmaceutical Industries Ltd., Israel; Teva Pharmaceuticals USA, Inc.
 SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006017357	A1	20060216	WO 2005-US24983	20050713
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,				

Updated Search

10509228

LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

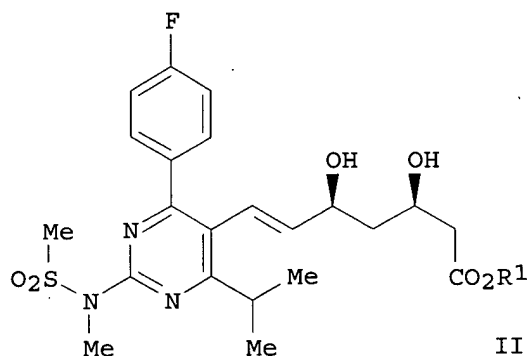
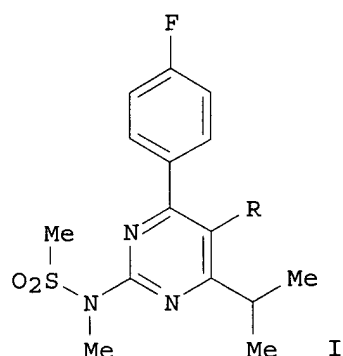
US 2006089501 A1 20060427 US 2005-181968 20050713
EP 1673351 A1 20060628 EP 2005-771256 20050713

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK,
BA, HR, IS, YU

PRIORITY APPLN. INFO.:

US 2004-587653P 20040713
WO 2005-US24983 20050713

GI



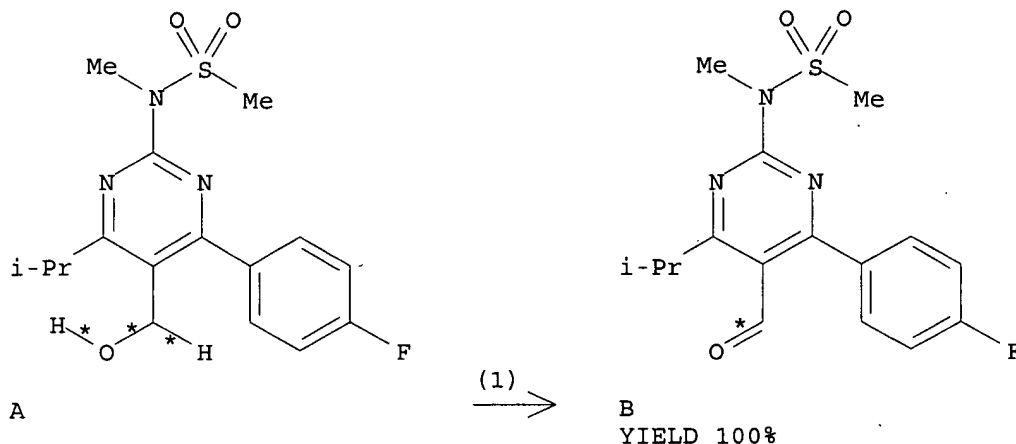
AB This invention provides a process for the preparation of the rosuvastatin intermediate I (R = CHO) by TEMPO-mediated oxidation of the corresponding alc. I (R = CH₂OH), and its subsequent conversion to rosuvastatin II (R₁ = H) and pharmaceutically acceptable salts thereof, such as II (R₁ = Na, 1/2Ca).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 11 A ==> B

Updated Search

10509228



RX(1) RCT A 147118-36-3
RGT C 2564-83-2 Me4-piperidoxyl, D 7681-52-9 NaOCl, E
7758-02-3 KBr
PRO B 147118-37-4
SOL 7732-18-5 Water, 75-05-8 MeCN
CON SUBSTAGE(1) 5 deg C
SUBSTAGE(3) 6 hours
NTE optimization study

L3 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 143:367114 CASREACT
TITLE: Total Synthesis of (-)-Kaitocephalin
AUTHOR(S): Kawasaki, Masanori; Shinada, Tetsuro; Hamada, Makoto;
Ohfuné, Yasufumi
CORPORATE SOURCE: Graduate School of Science, Osaka City University,
Sugimoto, Sumiyoshi, Osaka, 558-8585, Japan
SOURCE: Organic Letters (2005), 7(19), 4165-4167
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

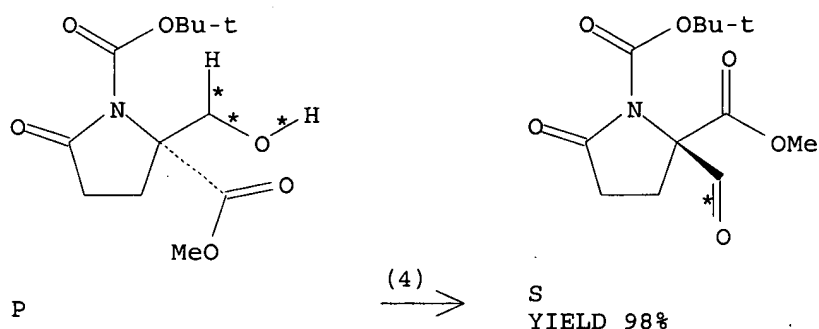
AB Total synthesis of the potent AMPA/KA receptor antagonist
(-)-kaitocephalin (I) and its three diastereomers has been accomplished.
The synthesis features strictly substrate-controlled operations to
 α -formylglutamate II starting with α -hydroxymethylglutamate.
The requisite 2R,3S,7R-stereocenters were efficiently constructed by
manipulation of stereoselective reactions: dihydroxylation of III followed
by azide substitution of the corresponding thionocarbonate IV and
Cu-mediated allylation of an acyliminium ion. All of the protecting
groups in V were removed simultaneously by $\text{AlCl}_3/\text{Me}_2\text{S}$ to give I.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

10509228

RX(4) OF 464 ...P ==> S...



RX(4) RCT P 866331-68-2
RGT T 2564-83-2 Me4-piperidoxyl, U 3240-34-4 PhI(OAc)2
PRO S 866331-49-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 26 hours, room temperature

L3 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:326257 CASREACT

TITLE: Theoretical and Experimental Design of Atypical Kinase Inhibitors: Application to p38 MAP Kinase

AUTHOR(S): McClure, Kim F.; Abramov, Yuriy A.; Laird, Ellen R.; Barberia, John T.; Cai, Weiling; Carty, Thomas J.; Cortina, Santo R.; Danley, Dennis E.; Dipesa, Alan J.; Donahue, Kathleen M.; Dombroski, Mark A.; Elliott, Nancy C.; Gabel, Christopher A.; Han, Seungil; Hynes, Thomas R.; LeMotte, Peter K.; Mansour, Mahmoud N.; Marr, Eric S.; Letavic, Michael A.; Pandit, Jayvardhan; Ripin, David B.; Sweeney, Francis J.; Tan, Douglas; Tao, Yong

CORPORATE SOURCE: Groton Laboratories, Pfizer Global Research and Development, Groton, CT, 06340, USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(18), 5728-5737

CODEN: JMCMAR; ISSN: 0022-2623

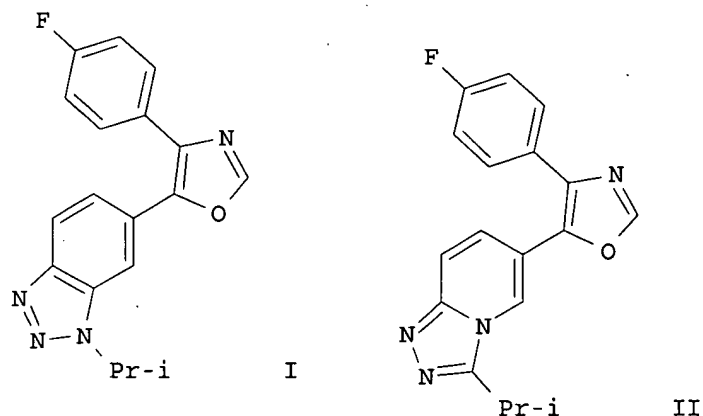
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

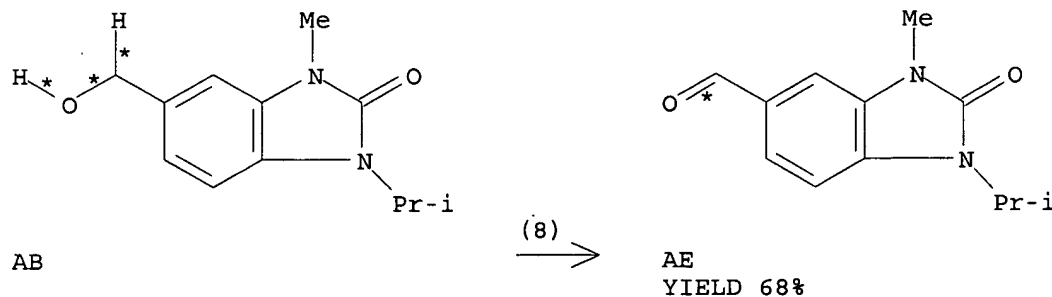
Updated Search



AB Mimics of the benzimidazolone nucleus found in inhibitors of p38 kinase are proposed, and their theor. potential as bioisosteres is described. A set of calculated descriptors relevant to the anticipated binding interaction for the fragments 1-methyl-1H-benzotriazole, 3-methylbenzo[d]isoxazole, and 3-methyl[1,2,4]triazolo[4,3-a]pyridine, pyridine, and 1,3-dimethyl-1,3-dihydro-benzoimidazol-2-one are reported. The design considerations and synthesis of p38 inhibitors based on these H-bond acceptor fragments is detailed. Comparative evaluation of the pyridine-, benzimidazolone-, benzotriazole-, and triazolopyridine-based inhibitors shows the triazoles I and II to be significantly more potent exptl. than the benzimidazolone after which they were modeled. An X-ray crystal structure of II bound to the active site shows that the triazole group serves as the H-bond acceptor but unexpectedly as a dual acceptor, inducing movement of the crossover connection of p38 α . The computed descriptors for the hydrophobic and π - π interaction capacities were the most useful in ranking potency.

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(8) OF 71 ...AB ==> AE...



RX(8) RCT AB 865443-84-1
 RGT AF 2564-83-2 Me4-piperidoxyl, AG 128-09-6
 Chlorosuccinimide, AH 1112-67-0 Bu4NC1
 PRO AE 865443-86-3
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2

Updated Search

10509228

CON 18 hours, 22 deg C, pH 8.6
NTE buffered solution, sodium bicarbonate-potassium carbonate

L3 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:229630 CASREACT

TITLE: Synthesis of Epoxyquinol A and Related Molecules:
Probing Chemical Reactivity of Epoxyquinol Dimers and
2H-Pyran Precursors

AUTHOR(S): Li, Chaomin; Porco, John A., Jr.

CORPORATE SOURCE: Department of Chemistry and Center for Chemical
Methodology and Library Development, Boston
University, Boston, MA, 02215, USA

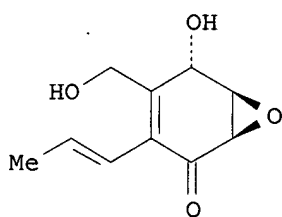
SOURCE: Journal of Organic Chemistry (2005), 70(15), 6053-6065
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

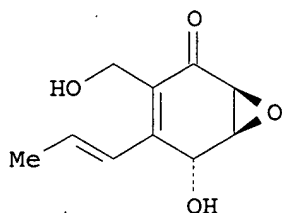
DOCUMENT TYPE: Journal

LANGUAGE: English

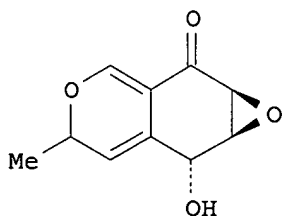
GI



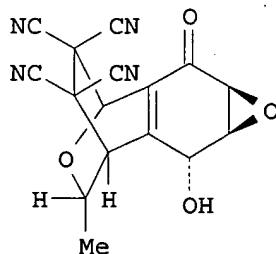
I



II



III



IV

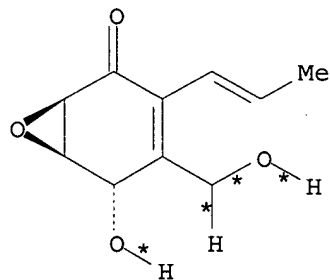
AB Total syntheses of the epoxyquinoid dimers, epoxyquinols A, B, and epoxytwinol A (RKB-3564 D), have been accomplished employing [4 + 2] and [4 + 4] dimerization of 2H-pyran epoxyquinol monomers, e.g. I. Modifications of 2H-pyran precursors have been explored, including alteration of epoxy alc. and diene stereochem. A stable 2H-pyran prepared by alteration of the epoxyquinol 2H-pyran nucleus was evaluated as a diene in Diels-Alder cycloaddn. with reactive dienophiles. Thus, reacting epoxyquinol II with Dess-Martin periodinane gave the 2H-pyran III which underwent Diels-Alder reaction with tetracyanoethylene to give adduct IV. Extensive studies for improving the [4 + 4] dimerization of selectively protected 2H-pyran monomers to afford the novel epoxyquinoid dimer epoxytwinol A were carried out, and valuable insight regarding competitive [4 + 2] and [4 + 4] dimerization processes has been obtained. In addition, chemical reactivities and structural modifications of epoxyquinol dimers have

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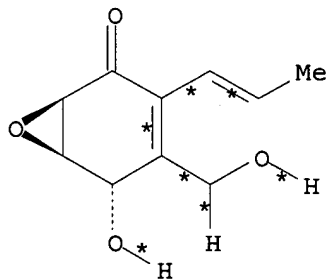
been evaluated, including [2 + 2] photocycloaddn. and [3,3] sigmatropic rearrangement, indicating the possibility for production of novel structural diversity from dimeric epoxyquinoid natural product frameworks.

REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

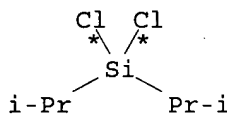
RX(25) OF 255 ...2 N + 2 BL ==> BM + BN...



N

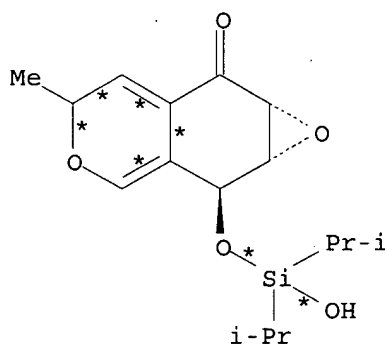


N

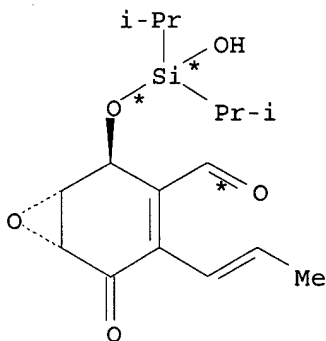


2 BL

(25)
→



BM
YIELD 76%



BN
YIELD 15%

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me4-piperidoxyl, X 7782-44-7 O2, Y
7758-89-6 CuCl
SOL 68-12-2 DMF
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4
RGT AY 288-32-4 1H-Imidazole
SOL 68-12-2 DMF

Updated Search

10509228

CON 15 minutes, 0 deg C

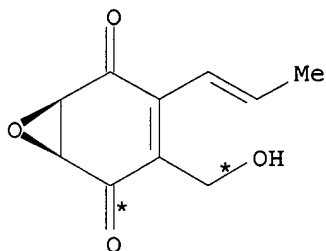
STAGE(3)

RGT L 7732-18-5 Water

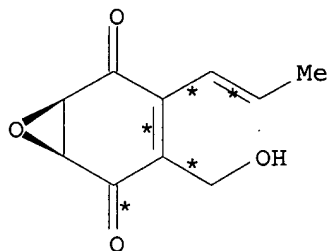
PRO BM 668987-33-5, BN 668987-32-4

RX(45) OF 255 COMPOSED OF RX(4), RX(25)

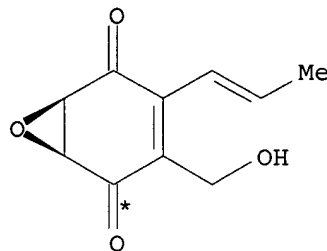
RX(45) 3 I + 2 BL ==> BM + BN



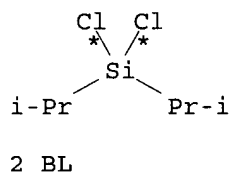
I



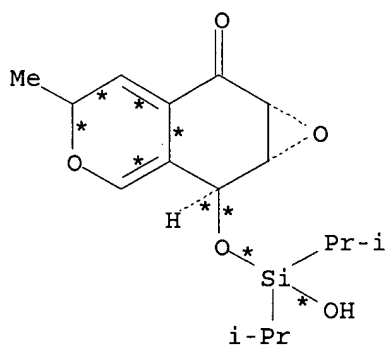
I



I

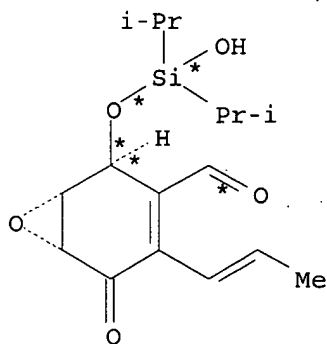


2
STEPS
→



BM
YIELD 76%

10509228



BN
YIELD 15%

RX(4) RCT I 473230-80-7

STAGE(1)

RGT P 1191-15-7 AlH(Bu-i)₂
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 10 minutes, -78 deg C

STAGE(2)

RGT Q 7647-01-0 HCl
SOL 7732-18-5 Water

PRO N 238424-94-7, O 862593-54-2
NTE stereoselective

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me₄-piperidoxyl, X 7782-44-7 O₂, Y
7758-89-6 CuCl
SOL 68-12-2 DMF
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4
RGT AY 288-32-4 1H-Imidazole
SOL 68-12-2 DMF
CON 15 minutes, 0 deg C

STAGE(3)

RGT L 7732-18-5 Water

PRO BM 668987-33-5, BN 668987-32-4

L3 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:229621 CASREACT

TITLE: Stereoselective synthesis of microcarpalide

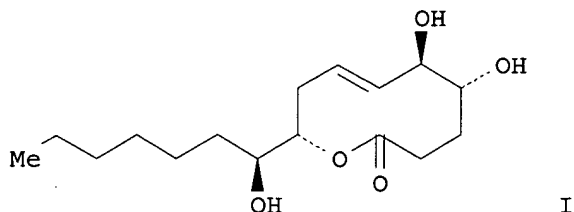
AUTHOR(S): Ishigami, Ken; Watanabe, Hidenori; Kitahara, Takeshi

CORPORATE SOURCE: Department of Applied Biological Chemistry, Graduate
School of Agricultural and Life Sciences, The

Updated Search

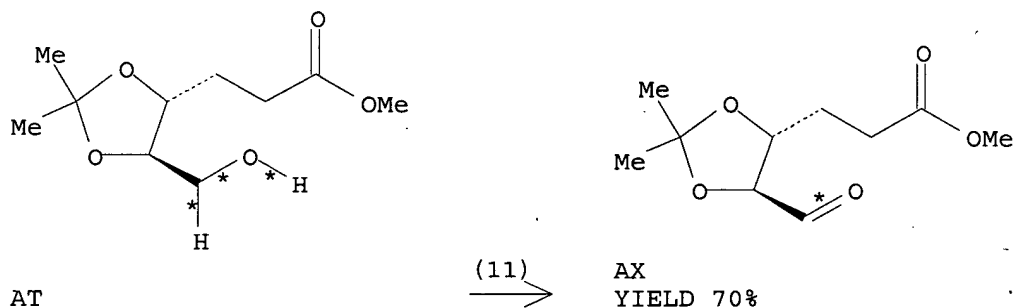
10509228

SOURCE: University of Tokyo, Bunkyo-ku, Tokyo, 113-8657, Japan
Tetrahedron (2005), 61(31), 7546-7553
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Microcarpalide (I) is a strong microfilament disrupting agent. The convergent and stereoselective synthesis of microcarpalide was succeeded via Julia olefination and macrolactonization.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 171 ...AT ==> AX...



RX(11) RCT AT 850222-14-9

STAGE(1)

RGT AY 95407-69-5 1-Piperidinyloxy,
4-methoxy-2,2,6,6-tetramethyl-, AZ 144-55-8 NaHCO₃, BA
7681-52-9 NaOCl, BB 7758-02-3 KBr
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 15 minutes, 0 deg C

STAGE(2)

RGT O 7772-98-7 Na₂S₂O₃
SOL 7732-18-5 Water

PRO AX 862907-39-9

Updated Search

10509228

L3 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:173109 CASREACT

TITLE: Total Synthesis of (-)-(α)-Kainic Acid via a Diastereoselective Methylenecyclopropane Ring Expansion

AUTHOR(S): Scott, Mark E.; Lautens, Mark

CORPORATE SOURCE: Davenport Research Laboratories, Department of Chemistry, University of Toronto, Toronto, ON, M5S 3H6, Can.

SOURCE: Organic Letters (2005), 7(14), 3045-3047

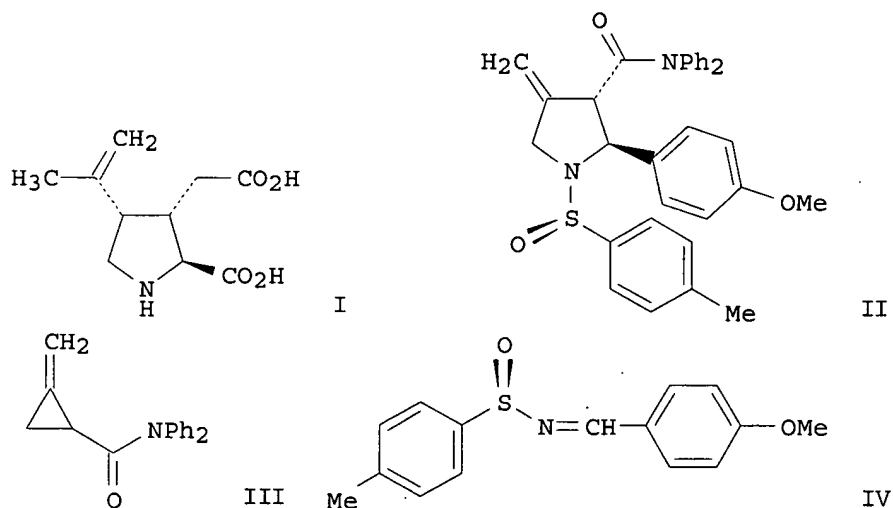
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



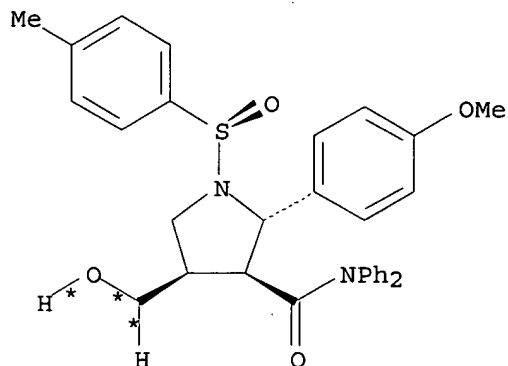
AB A concise and enantioselective synthesis of (-)- α -kainic acid (I) in 13 steps with an overall yield of 15% is reported. The kainoid precursor, (methylene)pyrrolidinyl amide II with the required C2/C3 trans stereochem., was prepared with excellent diastereoselectivity (>20:1) via a MgI₂-mediated ring expansion of methylenecyclopropyl amide III with chiral sulfinimine IV. A selective hydroboration was then employed to set the remaining stereochem. at the C4 position en route to I.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

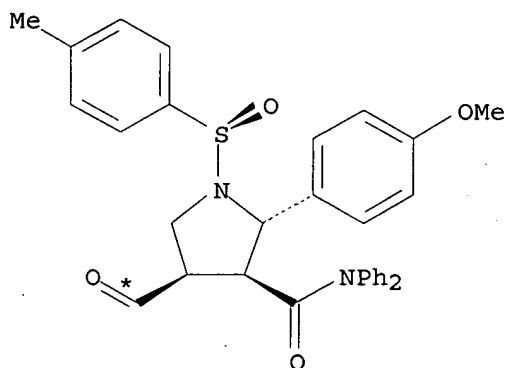
RX(3) OF 66 ...H ==> L...

Updated Search

10509228



H



L

YIELD 91%

RX(3) RCT H 861145-05-3

STAGE(1)

RGT M 2564-83-2 Me4-piperidoxyl, N 7647-15-6 NaBr
SOL 7732-18-5 Water, 108-88-3 PhMe, 141-78-6 AcOEt
CON room temperature -> 0 deg C

STAGE(2)

RGT O 144-55-8 NaHCO3, P 7681-52-9 NaOCl

PRO L 861145-06-4

L3 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:7520 CASREACT

TITLE: A total synthesis of the epoxyquinone based antifungal natural product (+)-ambuic acid

AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (2005), 46(17), 3045-3048

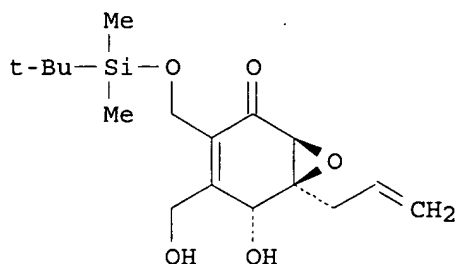
Updated Search

10509228

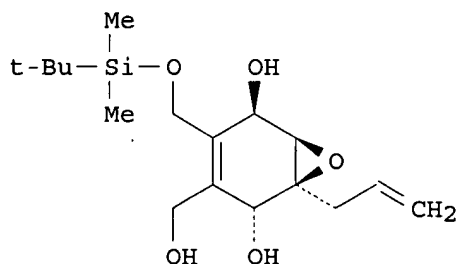
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
GI

Elsevier B.V.
Journal
English



I

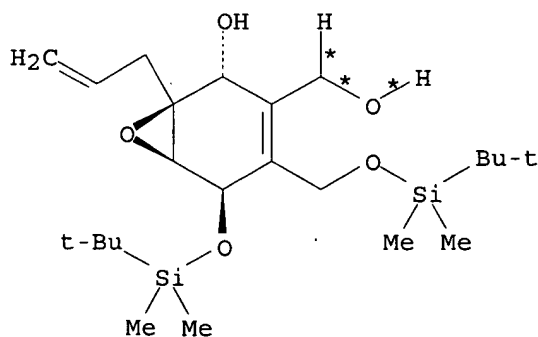


II

AB A total synthesis of the recently isolated polyketide natural product (+)-ambuic acid has been accomplished from the readily available Diels-Alder adduct of cyclopentadiene and 2-allyl-p-benzoquinone through a simple sequence with sound stereocontrol. An initial concern was to set the correct hydroxyl stereochem. at C7 in the evolution of epoxycyclohexanone I towards the natural product. This was accomplished by stereoselective NaBH₄ reduction of I with hydride addition from the face opposite to the epoxide ring which gave β-hydroxy compound II as the major product. II was then converted into the title compound

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

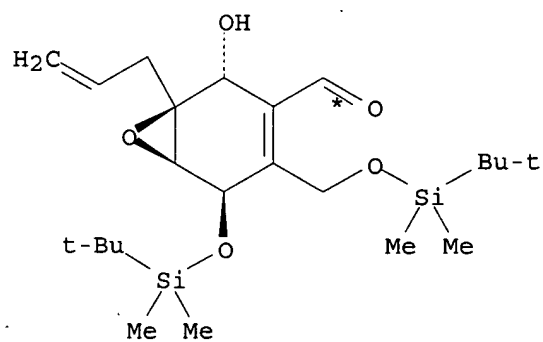
RX(5) OF 105 ...L ==> M...



L

(5) →

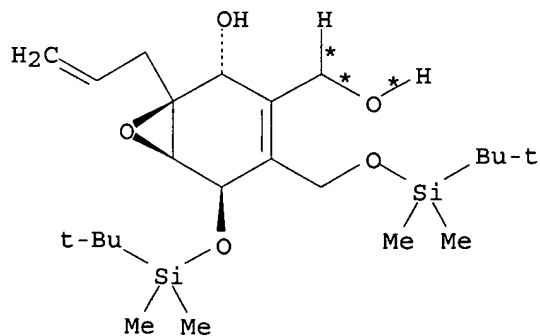
10509228



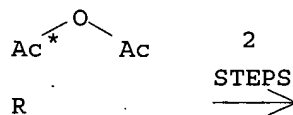
M
YIELD 90%

RX(5) RCT L 852392-89-3
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P
7758-89-6 CuCl
PRO M 852392-90-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(19) OF 105 COMPOSED OF RX(5), RX(6)
RX(19) L + R ==> S

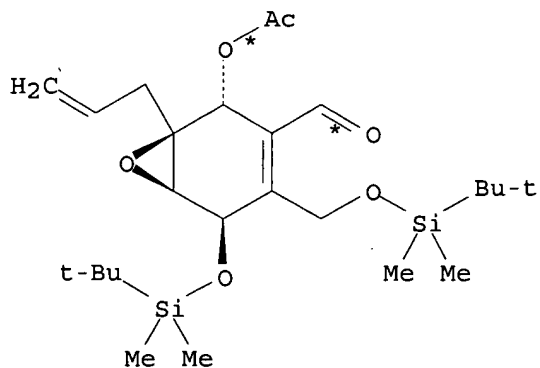


L



Updated Search

10509228

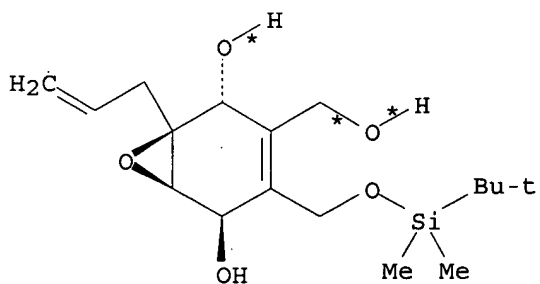


S
YIELD 98%

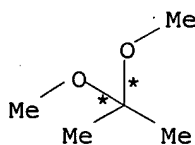
RX(5) RCT L 852392-89-3
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P
7758-89-6 CuCl
PRO M 852392-90-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(6) RCT M 852392-90-6, R 108-24-7
RGT T 110-86-1 Pyridine, U 1122-58-3 4-DMAP
PRO S 852392-91-7
SOL 75-09-2 CH2Cl2
CON 2.5 hours, 0 deg C

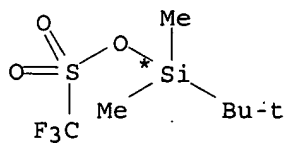
RX(32) OF 105 COMPOSED OF RX(2), RX(3), RX(4), RX(5)
RX(32) B + E + H ==> M



B



E

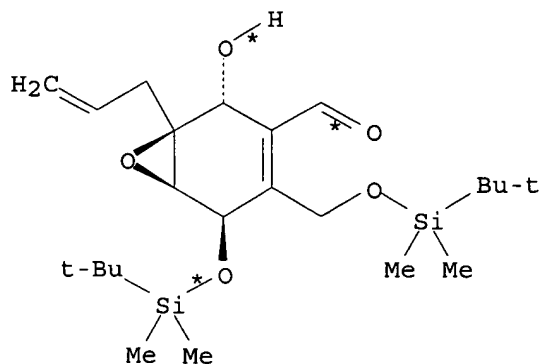


H

4
STEPS
→

Updated Search

10509228



M
YIELD 90%

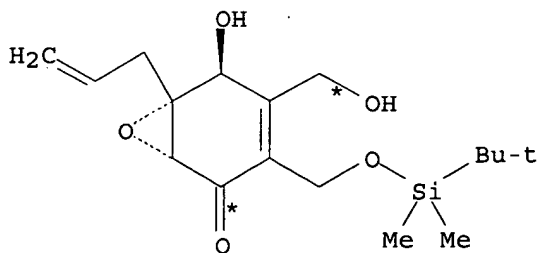
RX(2) RCT B 852392-86-0, E 77-76-9
RGT G 24057-28-1 Pyridinium tosylate
PRO F 852392-87-1
CON 5 hours, room temperature

RX(3) RCT F 852392-87-1, H 69739-34-0
RGT J 108-48-5 2,6-Lutidine
PRO I 852392-88-2
SOL 75-09-2 CH2Cl2
CON 15 minutes, 0 deg C

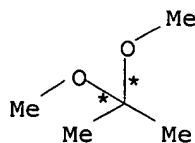
RX(4) RCT I 852392-88-2
RGT G 24057-28-1 Pyridinium tosylate
PRO L 852392-89-3
SOL 67-56-1 MeOH
CON 2 hours, room temperature

RX(5) RCT L 852392-89-3
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P
7758-89-6 CuCl
PRO M 852392-90-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(51) OF 105 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)
RX(51) A + E + H ==> M



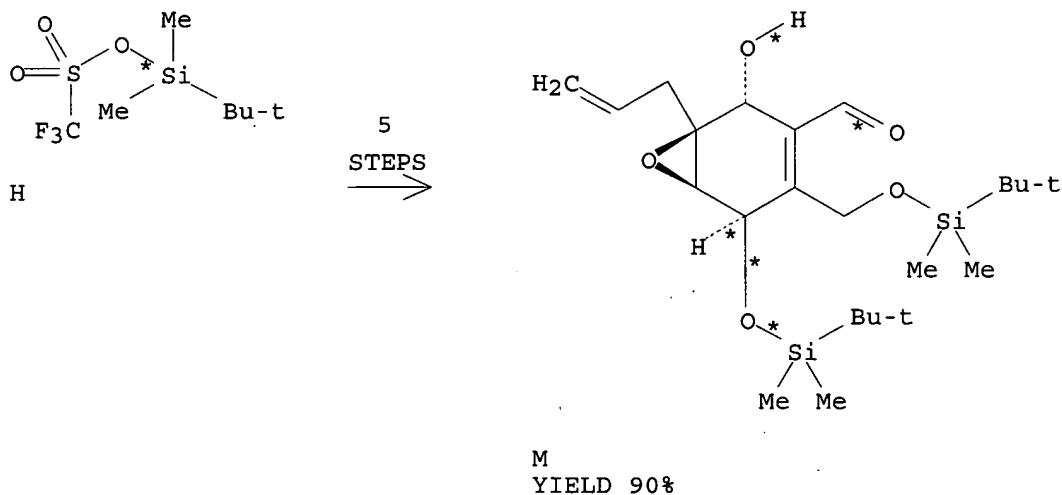
A



E

Updated Search

10509228

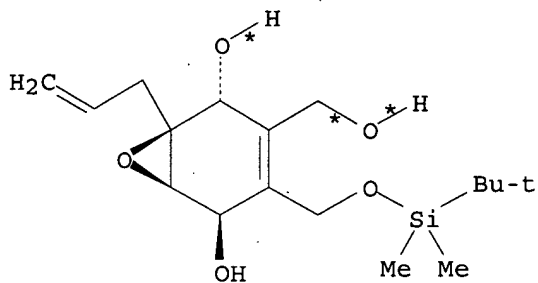


RX(1)	RCT	A 791854-39-2
	RGT	C 16940-66-2 NaBH4
	PRO	B 852392-86-0
	SOL	67-56-1 MeOH
	CON	10 minutes, -5 deg C
	NTE	stereoselective
RX(2)	RCT	B 852392-86-0, E 77-76-9
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	F 852392-87-1
	CON	5 hours, room temperature
RX(3)	RCT	F 852392-87-1, H 69739-34-0
	RGT	J 108-48-5 2,6-Lutidine
	PRO	I 852392-88-2
	SOL	75-09-2 CH2Cl2
	CON	15 minutes, 0 deg C
RX(4)	RCT	I 852392-88-2
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	L 852392-89-3
	SOL	67-56-1 MeOH
	CON	2 hours, room temperature
RX(5)	RCT	L 852392-89-3
	RGT	N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P 7758-89-6 CuCl
	PRO	M 852392-90-6
	SOL	68-12-2 DMF
	CON	3 hours, room temperature

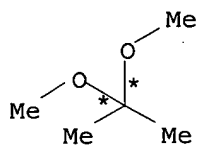
RX(52) OF 105 COMPOSED OF RX(2), RX(3), RX(4), RX(5), RX(6)
 RX(52) B + E + H + R ==> S

Updated Search

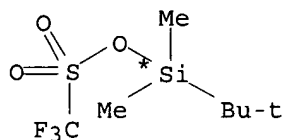
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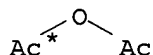
B



E

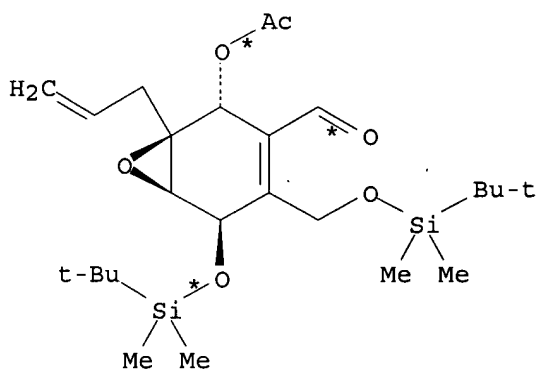


H



R

5
STEPS
→



S

YIELD 98%

RX(2) RCT B 852392-86-0, E 77-76-9
RGT G 24057-28-1 Pyridinium tosylate
PRO F 852392-87-1
CON 5 hours, room temperature

RX(3) RCT F 852392-87-1, H 69739-34-0
RGT J 108-48-5 2,6-Lutidine
PRO I 852392-88-2
SOL 75-09-2 CH₂Cl₂
CON 15 minutes, 0 deg C

RX(4) RCT I 852392-88-2
RGT G 24057-28-1 Pyridinium tosylate
PRO L 852392-89-3

Updated Search

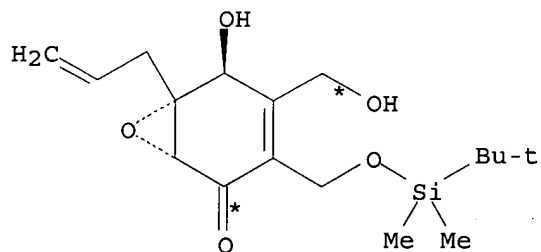
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SOL 67-56-1 MeOH
CON 2 hours, room temperature

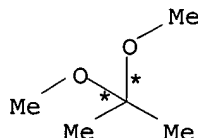
RX(5) RCT L 852392-89-3
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P
7758-89-6 CuCl
PRO M 852392-90-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(6) RCT M 852392-90-6, R 108-24-7
RGT T 110-86-1 Pyridine, U 1122-58-3 4-DMAP
PRO S 852392-91-7
SOL 75-09-2 CH2Cl2
CON 2.5 hours, 0 deg C

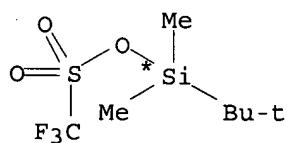
RX(53) OF 105 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)
RX(53) A + E + H + R ==> S



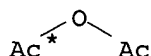
A



E



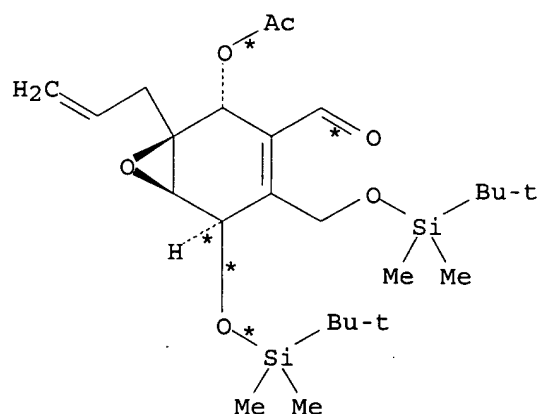
H



R

6
STEPS
→

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S

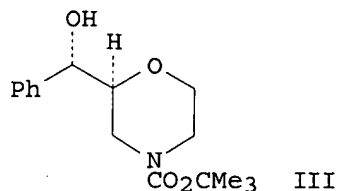
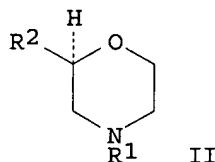
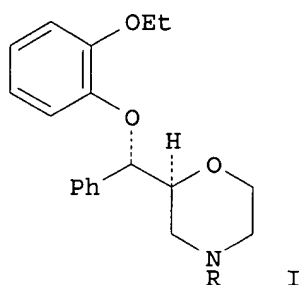
YIELD 98%

RX(1)	RCT	A 791854-39-2
	RGT	C 16940-66-2 NaBH4
	PRO	B 852392-86-0
	SOL	67-56-1 MeOH
	CON	10 minutes, -5 deg C
	NTE	stereoselective
RX(2)	RCT	B 852392-86-0, E 77-76-9
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	F 852392-87-1
	CON	5 hours, room temperature
RX(3)	RCT	F 852392-87-1, H 69739-34-0
	RGT	J 108-48-5 2,6-Lutidine
	PRO	I 852392-88-2
	SOL	75-09-2 CH2Cl2
	CON	15 minutes, 0 deg C
RX(4)	RCT	I 852392-88-2
	RGT	G 24057-28-1 Pyridinium tosylate
	PRO	L 852392-89-3
	SOL	67-56-1 MeOH
	CON	2 hours, room temperature
RX(5)	RCT	L 852392-89-3
	RGT	N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P 7758-89-6 CuCl
	PRO	M 852392-90-6
	SOL	68-12-2 DMF
	CON	3 hours, room temperature
RX(6)	RCT	M 852392-90-6, R 108-24-7
	RGT	T 110-86-1 Pyridine, U 1122-58-3 4-DMAP
	PRO	S 852392-91-7
	SOL	75-09-2 CH2Cl2
	CON	2.5 hours, 0 deg C

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L3 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:298056 CASREACT
TITLE: Asymmetric Synthesis of (+)-(S,S)-Reboxetine via a New
(S)-2-(Hydroxymethyl)morpholine Preparation
AUTHOR(S): Brenner, Eric; Baldwin, Ronald M.; Tamagnan, Gilles
CORPORATE SOURCE: Yale School of Medicine, VA Connecticut HCS, West
Haven, CT, 06516, USA
SOURCE: Organic Letters (2005), 7(5), 937-939
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Nonracemic (S,S)-reboxetine I (R = H) is prepared in eight steps and 30% overall yield; the key steps in the preparation of I are the selective oxidation of protected nonracemic hydroxymethylmorpholine II (R1 = Me₃COCO; R2 = CH₂OH) and nucleophilic aromatic substitution of the tricarbonylchromium complex of 1-ethoxy-2-fluorobenzene with nonracemic morpholinemethanol III. Chloroacetylation of (S)-3-amino-1,2-propanediol, regioselective cyclization mediated by potassium tert-butoxide in tert-amyl alc., reduction of the amide with Red-Al, and Boc protection of the morpholine nitrogen yields II (R1 = Me₃COCO; R2 = CH₂OH). Oxidation of II (R1 = Me₃COCO; R2 = CH₂OH) with TEMPO and trichloroisocyanuric acid in Et acetate with sodium bicarbonate yields II (R1 = Me₃COCO; R2 = OHC) in 89% yield; oxidation of a substrate lacking the Boc protecting group or oxidation of II (R1 = Me₃COCO; R2 = CH₂OH) by Swern reaction gives either no reaction or epimerization, while the use of Et acetate decreases chlorination byproducts and the use of sodium bicarbonate neutralizes hydrogen chloride generated from the trichloroisocyanuric acid. Addition of II (R1 = Me₃COCO; R2 = CHO) to diphenylzinc prepared from phenylmagnesium bromide and anhydrous zinc bromide

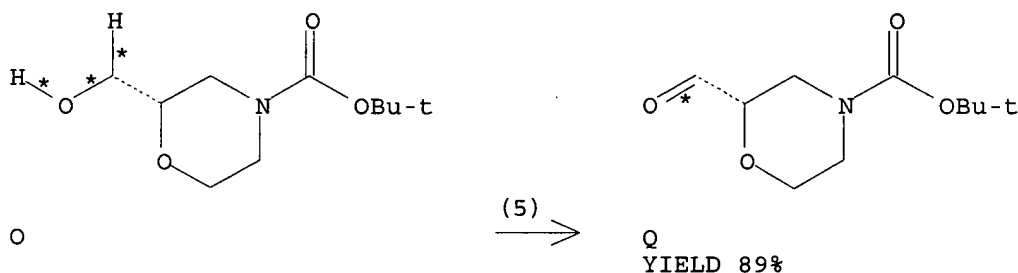
Updated Search

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in THF yields III in 60% yield in addition to 19% yield of the morpholinemethanol alc. epimer; the use of phenylmagnesium bromide as the nucleophile leads to aldehyde enolate formation and decreased yields of product. Nucleophilic aryl substitution of the tricarbonylchromium(0) complex of 1-ethoxy-2-fluorobenzene (prepared in two steps from 2-fluorophenol) with III and sodium hydride in DMF followed by oxidative demetalation with iodine in THF yields I (R = Me3COCO) in 95% yield; cleavage of the Boc group with TFA yields I (R = H). Mitsunobu reaction of the minor product of diphenylzinc addition to II (R1 = Me3COCO; R2 = OHC) with 2-ethoxyphenol followed by Boc cleavage also yields I (R = H); the yields of the Mitsunobu reaction do not exceed 53%.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 81 ...O ==> Q...



RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3
SOL 141-78-6 AcOEt
CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride
SOL 141-78-6 AcOEt
CON SUBSTAGE(1) 1 hour, -5 deg C
SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)2
SOL 7732-18-5 Water

PRO Q 847805-31-6

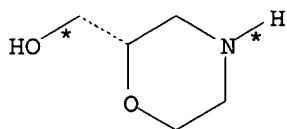
NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization, use of EtOAc suppresses chlorination

RX(15) OF 81 COMPOSED OF RX(4), RX(5)

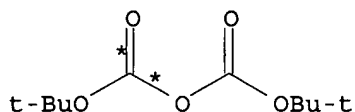
RX(15) K + N ==> Q

Updated Search

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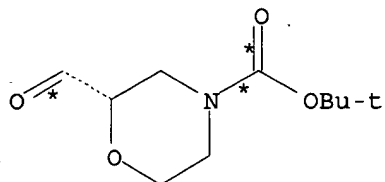


K



N

2
STEPS
→



Q

YIELD 89%

RX(4) RCT K 132073-83-7, N 24424-99-5
RGT P 1310-73-2 NaOH
PRO O 135065-76-8
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 3 hours, room temperature

RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3
SOL 141-78-6 AcOEt
CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride
SOL 141-78-6 AcOEt
CON SUBSTAGE(1) 1 hour, -5 deg C
SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)2
SOL 7732-18-5 Water

PRO Q 847805-31-6

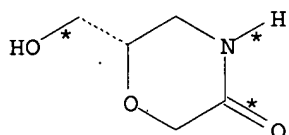
NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization,
use of EtOAc suppresses chlorination

RX(26) OF 81 COMPOSED OF RX(3), RX(4), RX(5).

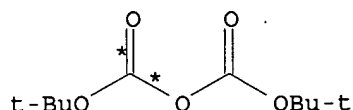
RX(26) G + N ==> Q

Updated Search

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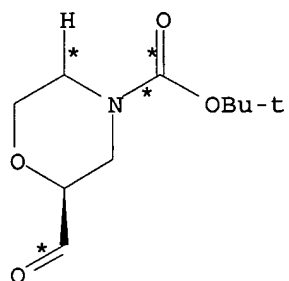


G



N

3
STEPS
→



Q

YIELD 89%

RX(3) RCT G 847805-30-5

STAGE(1)

RGT L 22722-98-1 Red-Al

SOL 109-99-9 THF

CON SUBSTAGE(1) 1 hour, 0 deg C

SUBSTAGE(2) 16 hours, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RGT I 7732-18-5 Water

PRO K 132073-83-7

RX(4) RCT K 132073-83-7, N 24424-99-5

RGT P 1310-73-2 NaOH

PRO O 135065-76-8

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 3 hours, room temperature

RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO3

SOL 141-78-6 AcOEt

CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) 1 hour, -5 deg C

SUBSTAGE(2) 1 hour, -5 deg C

Updated Search

STAGE(3)

RGT U 3375-31-3 Pd(OAc)₂

SOL 7732-18-5 Water

PRO Q 847805-31-6

NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization,
use of EtOAc suppresses chlorination

L3 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:176596 CASREACT

TITLE: Total Synthesis of Epoxyquinols A, B, and C and
Epoxytwinol A and the Reactivity of a 2H-Pyran
Derivative as the Diene Component in the Diels-Alder
ReactionAUTHOR(S): Shoji, Mitsuru; Imai, Hiroki; Mukaida, Makoto; Sakai,
Ken; Kakeya, Hideaki; Osada, Hiroyuki; Hayashi, YujiroCORPORATE SOURCE: Department of Industrial Chemistry, Faculty of
Engineering, Department of Applied Chemistry, Faculty
of Science, Tokyo University of Science, Shinjuku,
Tokyo, 162-8601, Japan

SOURCE: Journal of Organic Chemistry (2005), 70(1), 79-91

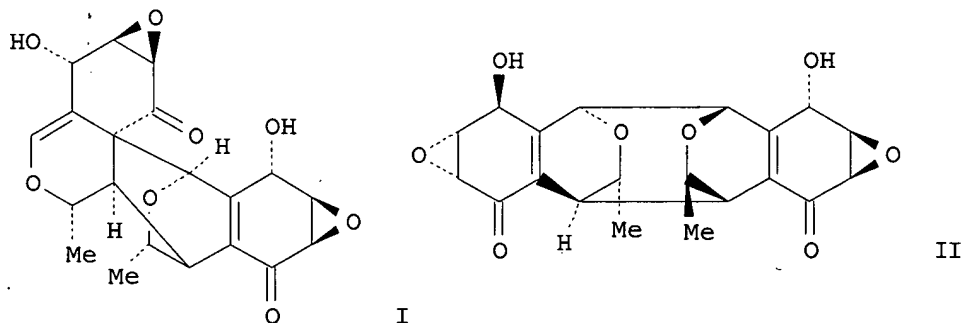
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



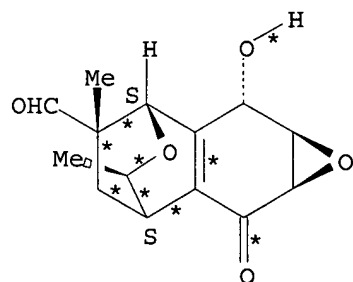
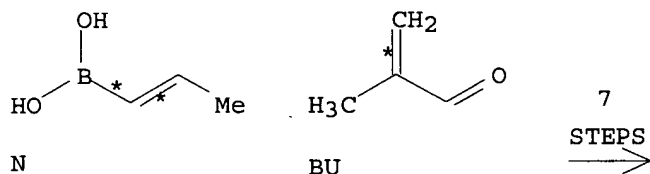
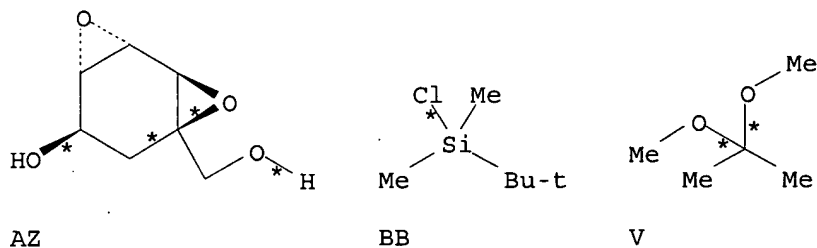
AB Full details of two versions of the total synthesis of epoxyquinols A, B, and C (I) and epoxytwinol A (II; RKB-3564D) are described. In the first-generation synthesis, the HfCl₄-mediated diastereoselective Diels-Alder reaction of furan with Corey's chiral auxiliary has been developed. In the second-generation synthesis, a chromatog.-free preparation of an iodolactone, by using acryloyl chloride as the dienophile in the Diels-Alder reaction of furan, and the lipase-mediated kinetic resolution of a cyclohexenol derivative have been developed. This second-generation synthesis is suitable for large-scale preparation. A biomimetic cascade reaction involving oxidation, 6 π -electrocyclization, and then Diels-Alder dimerization is the key reaction in the formation of the complex heptacyclic structure of epoxyquinols A, B, and C. Epoxytwinol A is synthesized by the cascade reaction composed of oxidation, 6 π -electrocyclization, and formal [4+4] cycloaddn. reactions. A

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2H-pyran, generated by oxidation/6 π -electrocyclization, acts as a good diene, reacting with several dienophiles to afford polycyclic compds. in one step. An azapentacyclic compound is synthesized by a similar cascade reaction composed of the four successive steps: oxidation, imine formation, 6 π -azaelectrocyclization, and Diels-Alder dimerization.

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(111) OF 236 COMPOSED OF RX(13), RX(5), RX(4), RX(14), RX(3), RX(15), RX(23)
 RX(111) AZ + BB + V + N + BU ==> BV



YIELD 69%

RX(13) RCT AZ 635678-63-6, BB 18162-48-6
 RGT BC 121-44-8 Et3N, BD 1122-58-3 4-DMAP
 PRO AA 488808-28-2
 SOL 75-09-2 CH2Cl2
 CON 15 hours, room temperature

RX(5) RCT AA 488808-28-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7758-02-3 KBr,

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AD 7681-52-9 NaOCl, AE 144-55-8 NaHCO₃
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 40 minutes, -10 deg C, pH 9.5

STAGE(2)

RGT AF 7631-86-9 SiO₂
SOL 108-88-3 PhMe
CON 4.5 hours, 70 deg C

PRO U 488808-29-3

RX(4) RCT U 488808-29-3

STAGE(1)

RGT X 9037-24-5 Amberlyst 15
SOL 67-56-1 MeOH
CON 5 hours, room temperature

STAGE(2)

RCT V 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
SOL 75-09-2 CH₂Cl₂
CON 4 hours, room temperature

PRO W 488808-30-6

RX(14) RCT W 488808-30-6
RGT AT 7553-56-2 I₂, BE 2712-78-9 PhI(O₂CCF₃)₂, BF 110-86-1 Pyridine
PRO M 488808-31-7
SOL 75-09-2 CH₂Cl₂
CON 22 hours, room temperature
NTE in the dark

RX(3) RCT M 488808-31-7, N 7547-97-9

STAGE(1)

CAT 14220-64-5 PdCl₂(PhCN)₂, 20667-12-3 Ag₂O, 603-32-7 Ph₃As
SOL 109-99-9 THF, 7732-18-5 Water
CON 11 hours, room temperature

STAGE(2)

RGT P 12125-02-9 NH₄Cl
SOL 7732-18-5 Water
CON 1 hour, room temperature

PRO O 238424-99-2
NTE in the dark

RX(15) RCT O 238424-99-2
RGT X 9037-24-5 Amberlyst 15
PRO G 238424-94-7
SOL 67-56-1 MeOH
CON 40 minutes, room temperature

RX(23) RCT G 238424-94-7

STAGE(1)

RGT K 1313-13-9 MnO₂
SOL 75-09-2 CH₂Cl₂

Updated Search

10509228

CON 1 hour, 0 deg C

STAGE(2)

RCT BU 78-85-3

CON room temperature

PRO BV 832731-77-8

NTE stereoselective

L3 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:424043 CASREACT

TITLE: Enantioselective total synthesis of epoxyquinone natural products (-)-phylllostine, (+)-epoxydon, (+)-epiepoxidon and (-)-panepophenanthrin: access to versatile chiral building blocks through enzymatic kinetic resolution

AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (2004), 45(41), 7683-7687

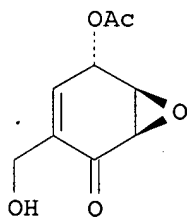
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier B.V.

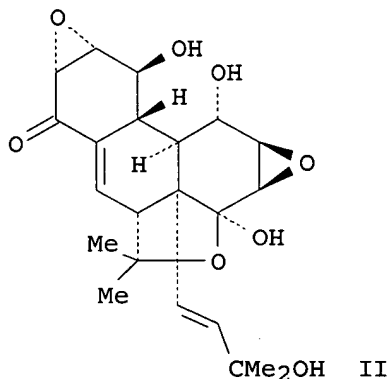
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

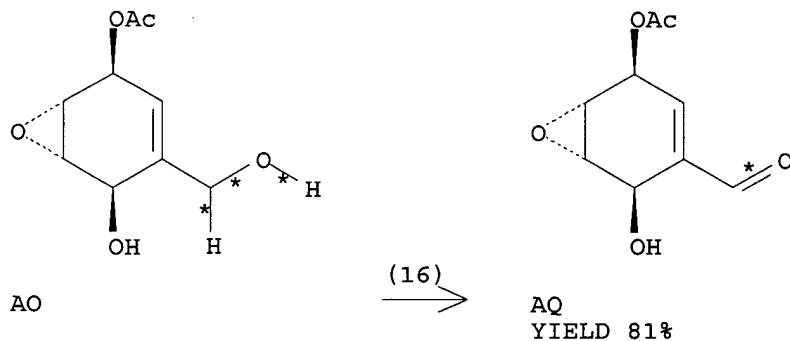
AB A new enzyme mediated protocol to access versatile chiral building blocks for the synthesis of epoxyquinone natural products is delineated. Total syntheses of (-)-phylllostine (I), (+)-epoxydon, (+)-epiepoxidon and (-)-panepophenanthrin (II) were accomplished to demonstrate the efficacy of this approach.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(16) OF 185 ...AO ==> AQ...

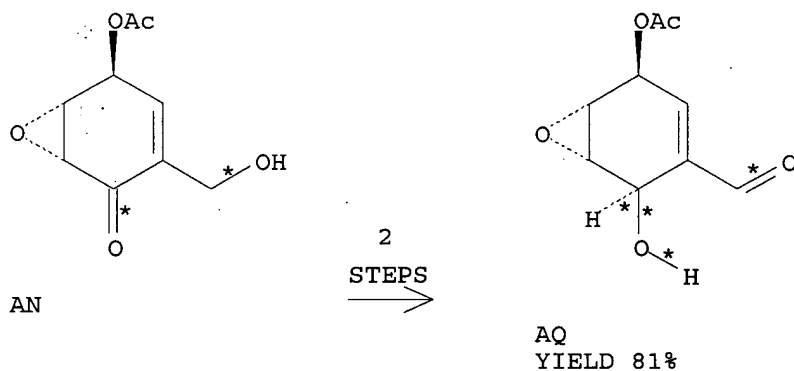
Updated Search

10509228



RX(16) RCT AO 792910-40-8
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT
7782-44-7 O2
PRO AQ 792910-42-0
SOL 68-12-2 DMF
CON room temperature

RX(36) OF 185 COMPOSED OF RX(15), RX(16)
RX(36) AN ==> AQ



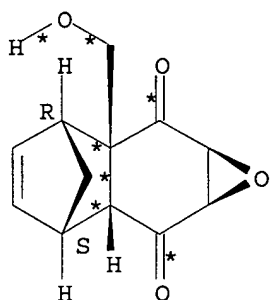
RX(15) RCT AN 792910-39-5
RGT AP 1191-15-7 AlH(Bu-i)2
PRO AO 792910-40-8
SOL 109-99-9 THF
CON -78 deg C

RX(16) RCT AO 792910-40-8
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT
7782-44-7 O2
PRO AQ 792910-42-0
SOL 68-12-2 DMF
CON room temperature

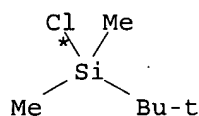
RX(116) OF 185 COMPOSED OF RX(6), RX(7), RX(8), RX(9), RX(14), RX(15), RX(16)
RX(116) P + R + Z ==> AQ

Updated Search

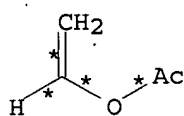
10509228



P

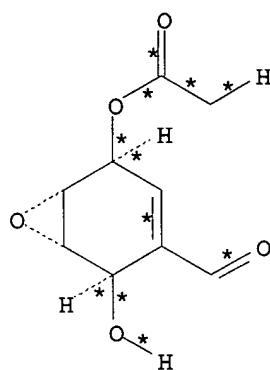


R



Z

7
STEPS
→



AQ

YIELD 81%

RX(6)	RCT	P 792910-31-7, R 18162-48-6
	RGT	T 288-32-4 1H-Imidazole
	PRO	S 792910-32-8
	CAT	1122-58-3 4-DMAP
	SOL	68-12-2 DMF
	CON	room temperature
RX(7)	RCT	S 792910-32-8
	RGT	X 16940-66-2 NaBH ₄
	PRO	W 792910-33-9
	SOL	67-56-1 MeOH
	CON	-15 deg C
RX(8)	RCT	W 792910-33-9, Z 108-05-4
	PRO	AA 792910-49-7, AB 792910-34-0
	CAT	9001-62-1 Lipase
	SOL	108-05-4 Vinyl acetate
	CON	room temperature
	NTE	enzymic
RX(9)	RCT	AB 792910-34-0
	PRO	AD 792910-35-1
	SOL	101-84-8 PhOPh

Updated Search

10509228

CON 5 minutes, 240 deg C

RX(14) RCT AD 792910-35-1
RGT C 62778-11-4 Olah's reagent
PRO AN 792910-39-5
SOL 109-99-9 THF
CON 0 deg C

RX(15) RCT AN 792910-39-5
RGT AP 1191-15-7 AlH(Bu-i)₂
PRO AO 792910-40-8
SOL 109-99-9 THF
CON -78 deg C

RX(16) RCT AO 792910-40-8
RGT AR 2564-83-2 Me4-piperidoxyl, AS 7758-89-6 CuCl, AT
7782-44-7 O₂
PRO AQ 792910-42-0
SOL 68-12-2 DMF
CON room temperature

L3 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:410727 CASREACT

TITLE: Total Synthesis of the Novel, Biologically Active
Epoxyquinone Dimer (+)-Torreyanic Acid: A
Biomimetic Approach

AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of
Science, Bangalore, 560 012, India

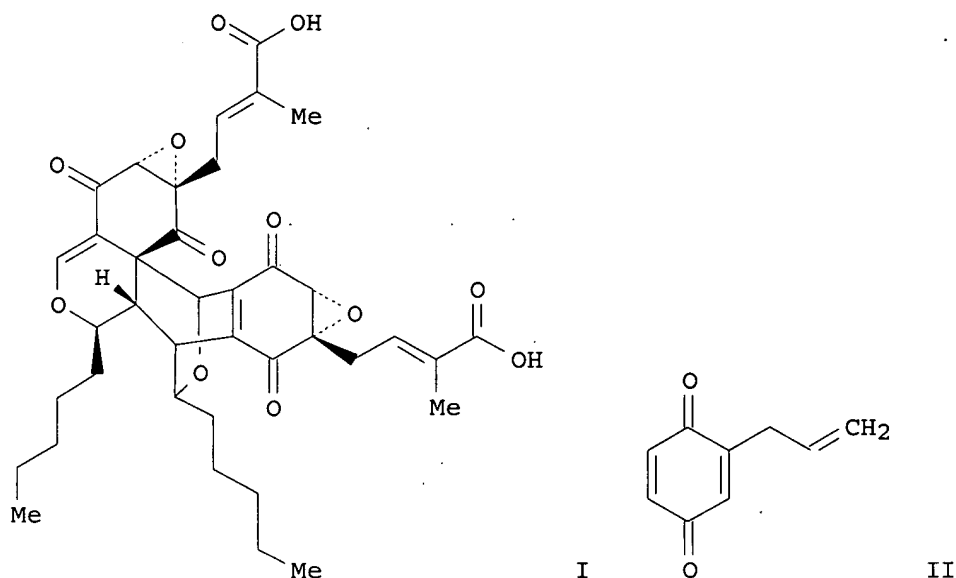
SOURCE: Organic Letters (2004), 6(22), 3985-3988
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

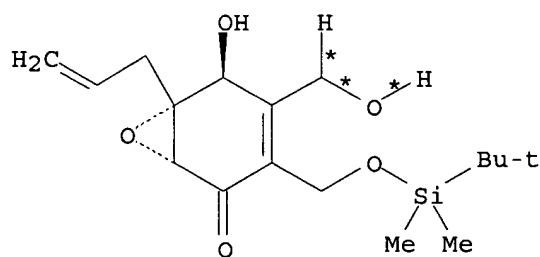
GI



AB A total synthesis of the complex, biol. active, dimeric natural product (\pm)-torreyanic acid (I), which is composed of seven rings and laced with dense oxy-functionalization, has been accomplished from readily available allyl-substituted p-benzoquinone II. Our synthetic stratagem involves crafting an epoxyquinone monomer for use in a biomimetic cascade process involving a tandem 6π electrocyclization and a Diels-Alder dimerization.

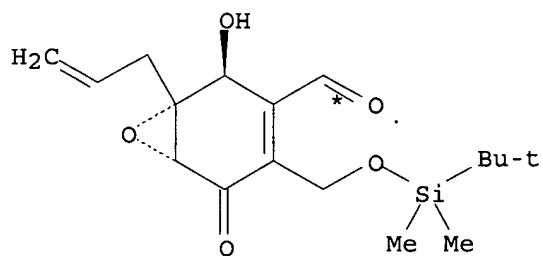
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 230 ...Y ==> AA...



(9) \longrightarrow

10509228



AA
YIELD 90%

RX(9) RCT Y 791854-39-2

STAGE(1)

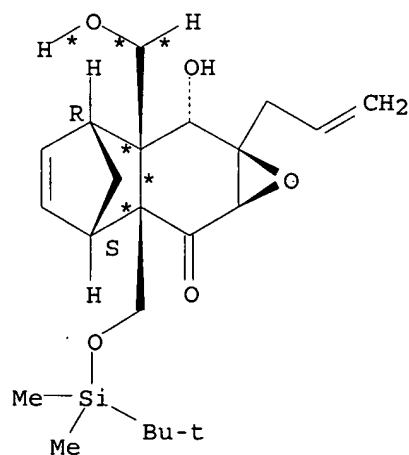
RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

PRO AA 791854-32-5
NTE chemoselective

RX(29) OF 230 COMPOSED OF RX(8), RX(9)
RX(29) W ==> AA

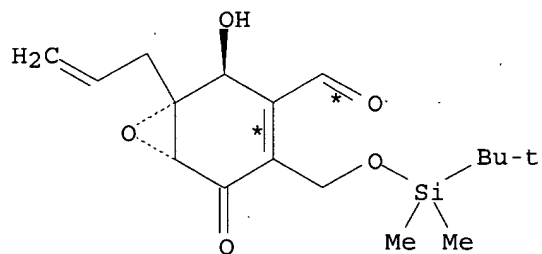


W

2
STEPS
→

Updated Search

10509228



AA

YIELD 90%

RX(8) RCT W 791854-38-1
RGT Z 101-84-8 PhOPh
PRO Y 791854-39-2
CON 6 minutes, 220 deg C
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

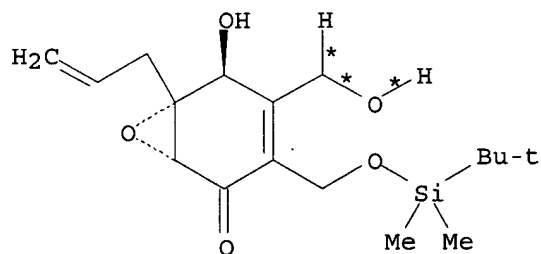
STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

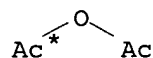
PRO AA 791854-32-5
NTE chemoselective

RX(30) OF 230 COMPOSED OF RX(9), RX(10)

RX(30) Y + AE ==> AF



Y

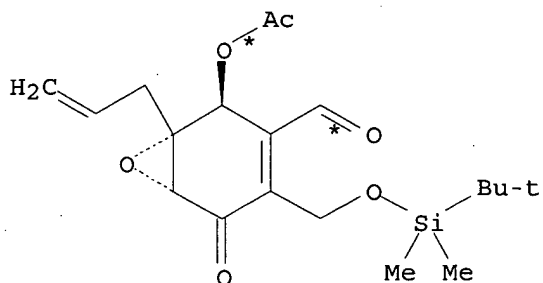


AE

2
STEPS
→

Updated Search

10509228



AF
YIELD 98%

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

PRO AA 791854-32-5
NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

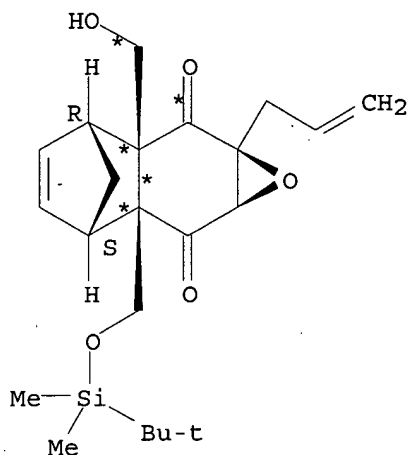
RGT D 7732-18-5 Water

PRO AF 791854-40-5

RX(53) OF 230 COMPOSED OF RX(7), RX(8), RX(9)

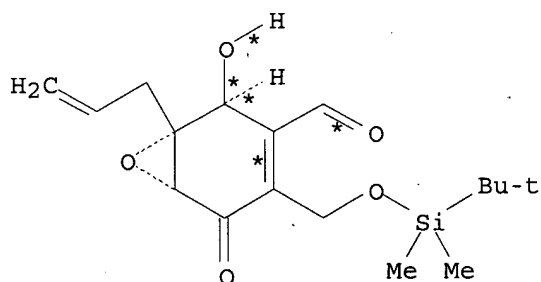
RX(53) V ==> AA

10509228



V

3
STEPS
→



AA

YIELD 90%

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH₄

SOL 67-56-1 MeOH

CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1

NTE regioselective, stereoselective

RX(8)

RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

NTE retro Diels-Alder reaction

RX(9)

RCT Y 791854-39-2

Updated Search

10509228

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

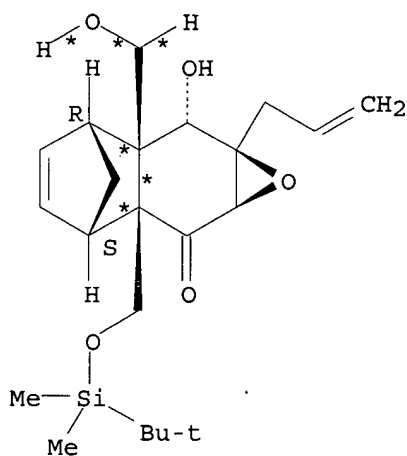
SOL 7732-18-5 Water

PRO AA 791854-32-5

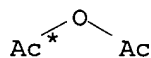
NTE chemoselective

RX(55) OF 230 COMPOSED OF RX(8), RX(9), RX(10)

RX(55) W + AE ==> AF

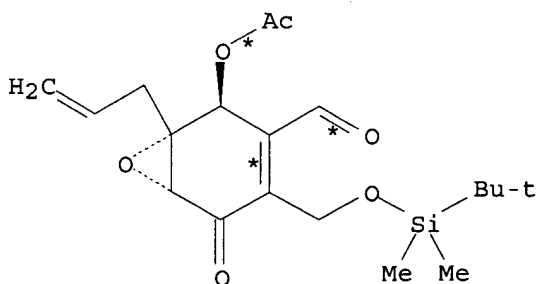


W



AE

3
STEPS
→



AF

YIELD 98%

RX(8)

RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

Updated Search

10509228

NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4

SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

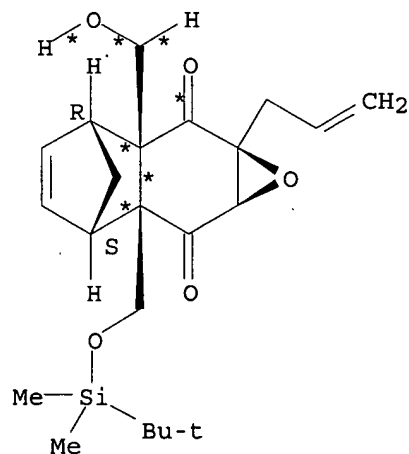
STAGE(2)

RGT D 7732-18-5 Water

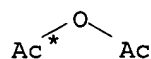
PRO AF 791854-40-5

RX(56) OF 230 COMPOSED OF RX(7), RX(8), RX(9), RX(10)

RX(56) V + AE ==> AF



V

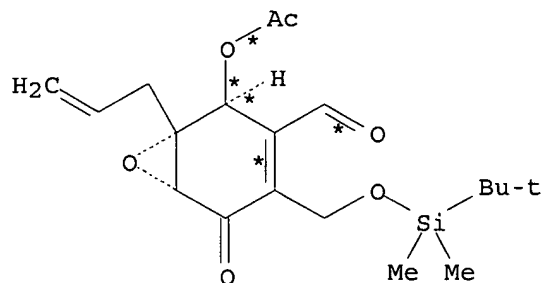


AE

4
STEPS
→

Updated Search

10509228



AF
YIELD 98%

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH₄

SOL 67-56-1 MeOH

CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1

NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1

RGT Z 101-84-8 PhOPh

PRO Y 791854-39-2

CON 6 minutes, 220 deg C

NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me₄-piperidoxyl, AC 7681-65-4 CuI

SOL 68-12-2 DMF

CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO₄

SOL 7732-18-5 Water

PRO AA 791854-32-5

NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

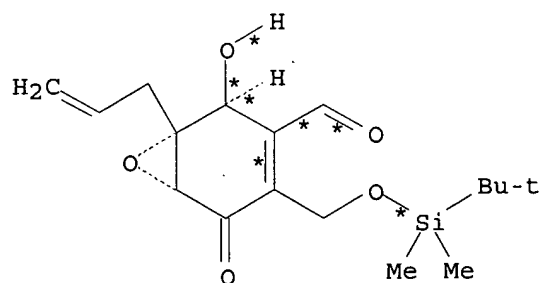
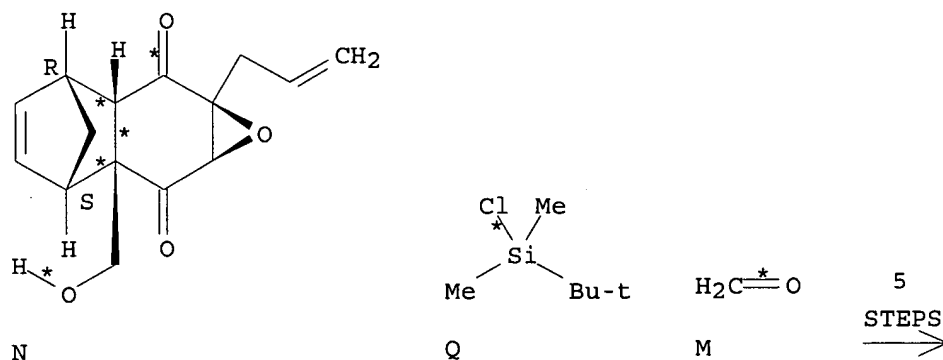
RGT D 7732-18-5 Water

Updated Search

10509228

PRO AF 791854-40-5

RX(89) OF 230 COMPOSED OF RX(5), RX(6), RX(7), RX(8), RX(9)
RX(89) N + Q + M ==> AA



AA
YIELD 90%

RX(5) RCT N 791854-36-9, Q 18162-48-6

STAGE(1)

RGT S 288-32-4 1H-Imidazole
CAT 1122-58-3 4-DMAP
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water
CON room temperature

PRO R 791854-37-0

RX(6) RCT R 791854-37-0

STAGE(1)

RGT O 6674-22-2 DBU

Updated Search

10509228

SOL 109-99-9 THF
CON 1 hour, 0 deg C

STAGE(2)

RCT M 50-00-0
SOL 7732-18-5 Water
CON 36 hours, room temperature

PRO V 791854-33-6
NTE stereoselective

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH4
SOL 67-56-1 MeOH
CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1
NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1
RGT Z 101-84-8 PhOPh
PRO Y 791854-39-2
CON 6 minutes, 220 deg C
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

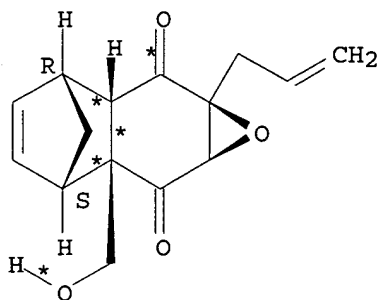
STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

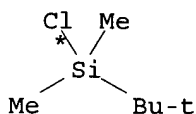
PRO AA 791854-32-5
NTE chemoselective

RX(94) OF 230 COMPOSED OF RX(5), RX(6), RX(7), RX(8), RX(9), RX(10)
RX(94) N + Q + M + AE ==> AF

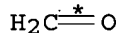
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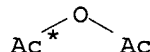
N



Q

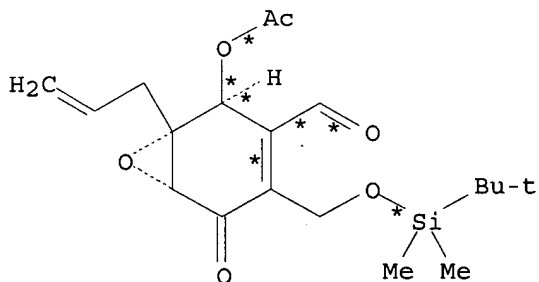


M



AE

6
STEPS
→



AF

YIELD 98%

RX(5) RCT N 791854-36-9, Q 18162-48-6

STAGE(1)

RGT S 288-32-4 1H-Imidazole

CAT 1122-58-3 4-DMAP

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water

CON room temperature

PRO R 791854-37-0

RX(6) RCT R 791854-37-0

STAGE(1)

RGT O 6674-22-2 DBU

SOL 109-99-9 THF

CON 1 hour, 0 deg C

Updated Search

10509228

STAGE(2)

RCT M 50-00-0
SOL 7732-18-5 Water
CON 36 hours, room temperature

PRO V 791854-33-6
NTE stereoselective

RX(7) RCT V 791854-33-6

STAGE(1)

RGT X 16940-66-2 NaBH4
SOL 67-56-1 MeOH
CON 1 hour, -5 deg C

STAGE(2)

RGT D 7732-18-5 Water

PRO W 791854-38-1
NTE regioselective, stereoselective

RX(8) RCT W 791854-38-1
RGT Z 101-84-8 PhOPh
PRO Y 791854-39-2
CON 6 minutes, 220 deg C
NTE retro Diels-Alder reaction

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

PRO AA 791854-32-5
NTE chemoselective

RX(10) RCT AA 791854-32-5, AE 108-24-7

STAGE(1)

CAT 110-86-1 Pyridine, 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 3 hours, room temperature

STAGE(2)

RGT D 7732-18-5 Water

PRO AF 791854-40-5

L3 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:410671 CASREACT

TITLE: The oxidation of alcohols in N-Oxyl-immobilized silica

Updated Search

10509228

gel/aqueous NaOCl disperse systems. A prominent access to a column-flow system

AUTHOR(S): Tanaka, Hideo; Chou, Jingyu; Mine, Machiko; Kuroboshi, Manabu

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Okayama University, Okayama, 700-8530, Japan

SOURCE: Bulletin of the Chemical Society of Japan (2004), 77(9), 1745-1755
CODEN: BCSJA8; ISSN: 0009-2673

PUBLISHER: Chemical Society of Japan

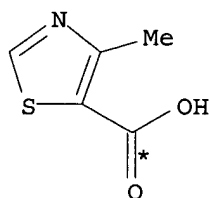
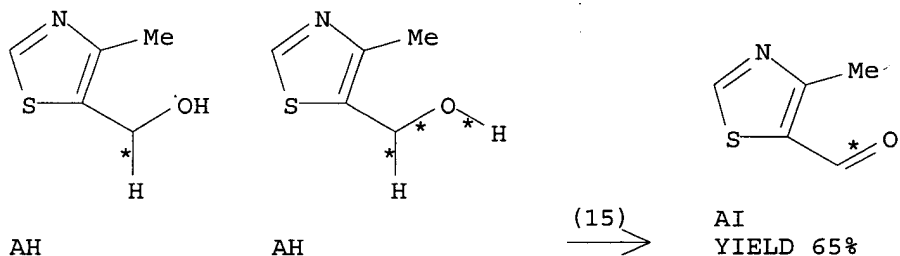
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The oxidation of alcs. was performed successfully in a disperse system with N-oxyl-adsorbed or immobilized silica gel as a disperse phase and aqueous NaOCl as a disperse medium. In the disperse system, the oxidation of sec-alcs. afforded the corresponding ketones, while prim-alcs. were oxidized to aldehydes and/or carboxylic acids depending on their structures and reaction conditions. The N-oxyl-immobilized silica gel was recovered and repeatedly used without a significant change in the product yields. A column-flow system was also investigated for the oxidation of alcs. by use of a newly devised column packed with the N-oxyl-immobilized silica gel.

REFERENCE COUNT: 142 THERE ARE 142 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(15) OF 33 2 AH ==> AI + AJ



AJ
YIELD 11%

RX(15) RCT AH 1977-06-6

STAGE(1)

RGT C 3225-26-1 Piperidinoxy deriv., D 7631-86-9

Updated Search

10509228

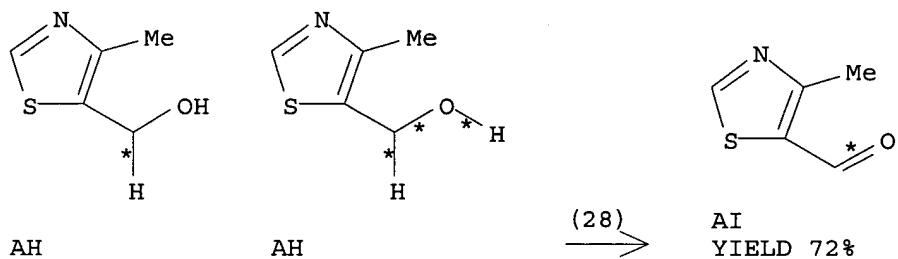
SiO2
SOL 67-64-1 Me2CO
CON 10 minutes, room temperature

STAGE(2)

RGT E 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

RX(28) OF 33 2 AH ==> AI + AJ



AJ
YIELD 15%

RX(28) RCT AH 1977-06-6

STAGE(1)

RGT AU 21216-79-5D 1-Piperidinyloxy,
4-[(aminocarbonyl)amino]-2,2,6,6-tetramethyl-
SOL 67-64-1 Me2CO
CON 10 minutes, room temperature

STAGE(2)

RGT E 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0.5 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

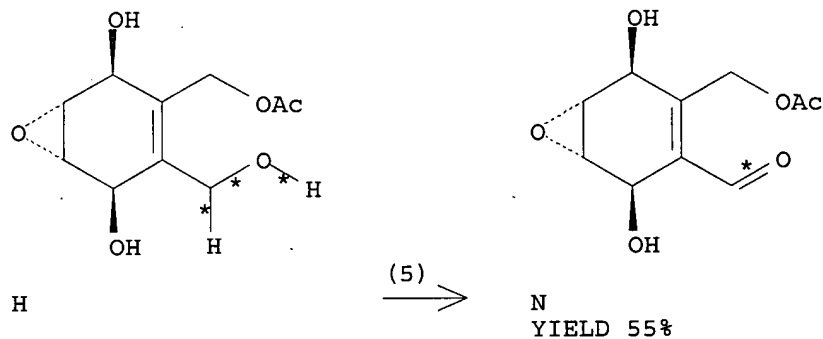
L3 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

ACCESSION NUMBER: 141:206943 CASREACT
TITLE: Enantioselective Total Synthesis of (+)-Eupenoxide and (+)-Phomoxide: Revision of Structures and Assignment of Absolute Configuration
AUTHOR(S): Mehta, Goverdhan; Roy, Subhrangsu
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India
SOURCE: Organic Letters (2004), 6(14), 2389-2392
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Stereo- and enantioselective total syntheses of the novel, polyketide natural products ent-eupenoxide and ent-phomoxide were accomplished from the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone. These synthetic studies necessitate the revision of the assigned stereostructures of the natural products and reveal their absolute configuration.
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

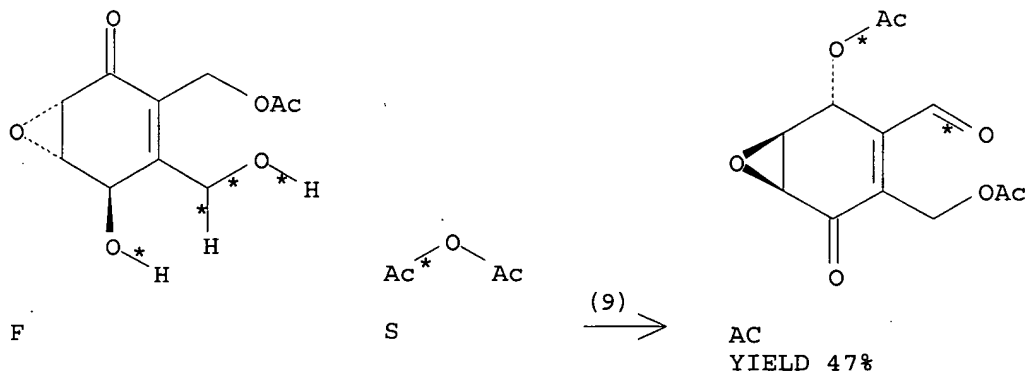
RX(5) OF 87 ...H ==> N...



RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(9) OF 87 ...F + S ==> AC...

10509228



RX(9) RCT F 676263-76-6

STAGE(1)

RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl

SOL 68-12-2 DMF

STAGE(2)

RCT S 108-24-7

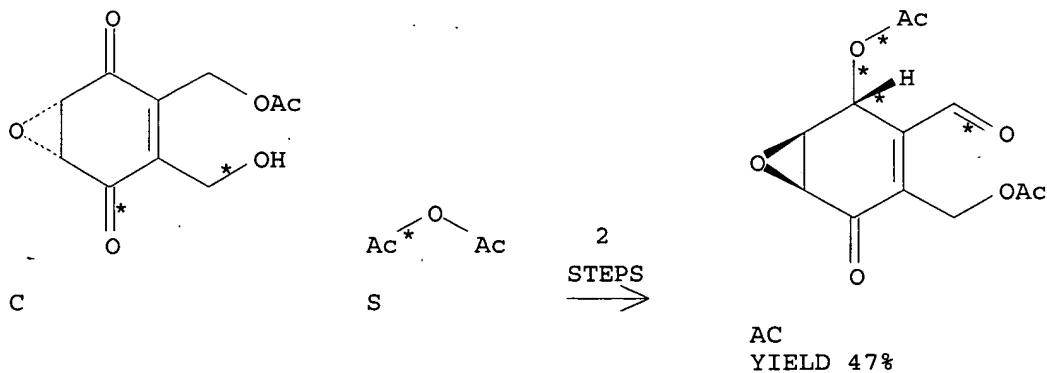
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

PRO AC 676263-80-2

RX(21) OF 87 COMPOSED OF RX(2), RX(9)

RX(21) C + S ==> AC



RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)2
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(9) RCT F 676263-76-6

Updated Search

10509228

STAGE(1)

RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
SOL 68-12-2 DMF

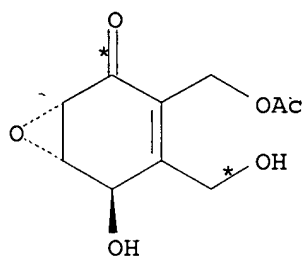
STAGE(2)

RCT S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2

PRO AC 676263-80-2

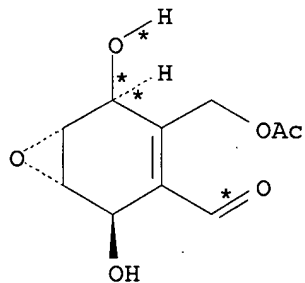
RX(23) OF 87 COMPOSED OF RX(3), RX(5)

RX(23) F ==> N



F

2
STEPS
→



N

YIELD 55%

RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

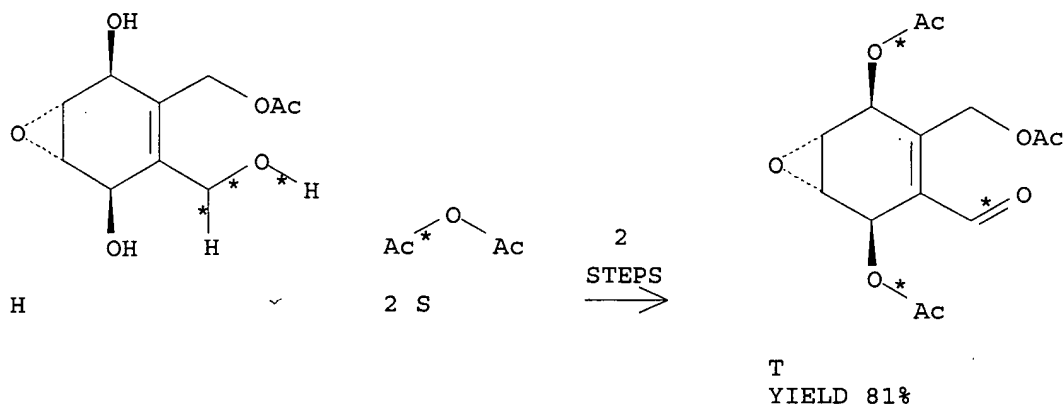
RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

Updated Search

10509228

RX(24) OF 87 COMPOSED OF RX(5), RX(6)

RX(24) H + 2 S ==> T

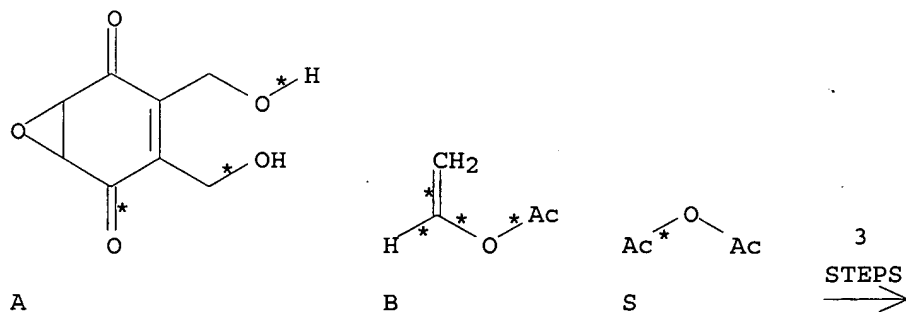


RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
PRO T 735317-28-9
SOL 75-09-2 CH2Cl2

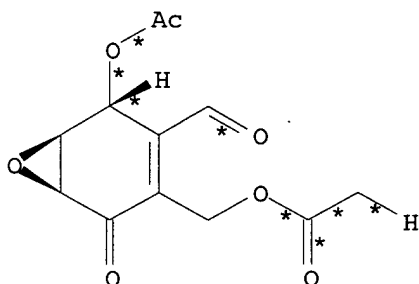
RX(37) OF 87 COMPOSED OF RX(1), RX(2), RX(9)

RX(37) A + B + S ==> AC



Updated Search

10509228



AC
YIELD 47%

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 109-99-9 THF
CON 0 deg C
NTE biotransformation, enzymic(lipase PS)

RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)₂
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(9) RCT F 676263-76-6

STAGE(1)

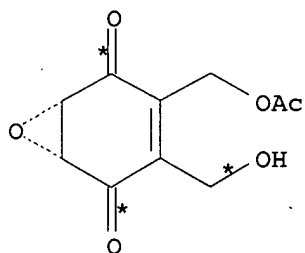
RGT O 2564-83-2 Me₄-piperidoxyl, P 7782-44-7 O₂, Q
7758-89-6 CuCl
SOL 68-12-2 DMF

STAGE(2)

RCT S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂

PRO AC 676263-80-2

RX(39) OF 87 COMPOSED OF RX(2), RX(3), RX(5)
RX(39) C ==> N

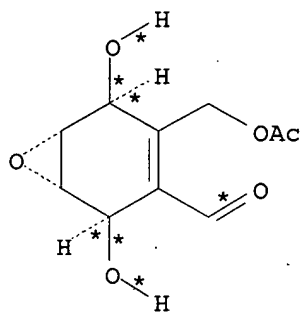


C

3
STEPS
→

Updated Search

10509228



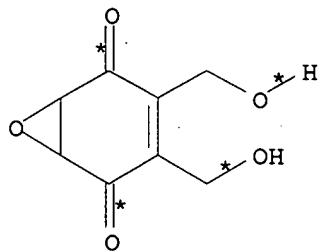
N
YIELD 55%

RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)2
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

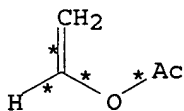
RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(43) OF 87 COMPOSED OF RX(1), RX(2), RX(3), RX(5)
RX(43) A + B ==> N



A

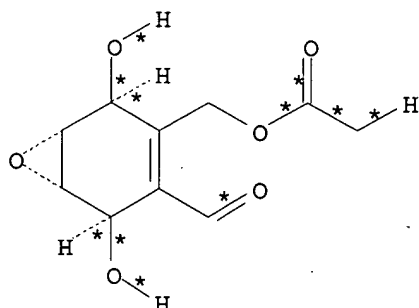


B

4
STEPS
→

Updated Search

10509228



N
YIELD 55%

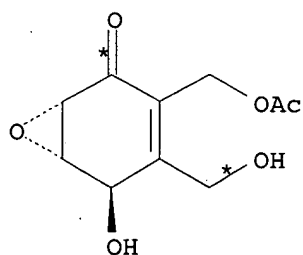
RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 109-99-9 THF
CON 0 deg C
NTE biotransformation, enzymic(lipase PS)

RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)2
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

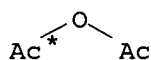
RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(46) OF 87 COMPOSED OF RX(3), RX(5), RX(6)
RX(46) F + 2 S ==> T



F

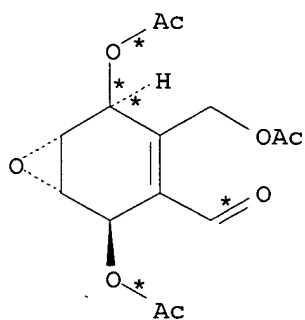


2 S

3
STEPS
→

Updated Search

10509228



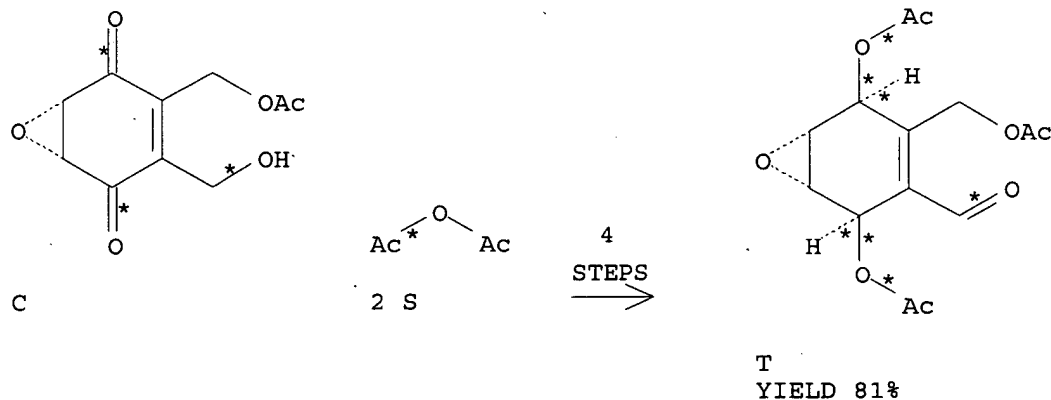
T
YIELD 81%

RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH₄, J 7790-86-5 CeCl₃
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me₄-piperidoxyl, P 7782-44-7 O₂, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
PRO T 735317-28-9
SOL 75-09-2 CH₂Cl₂

RX(47) OF 87 COMPOSED OF RX(2), RX(3), RX(5), RX(6)
RX(47) C + 2 S ==> T



RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)₂

Updated Search

10509228

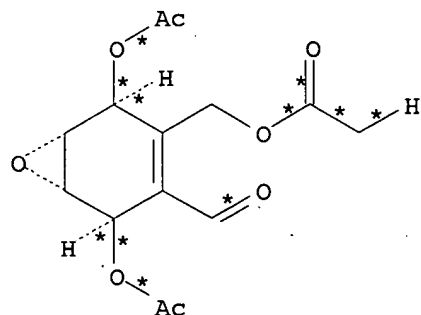
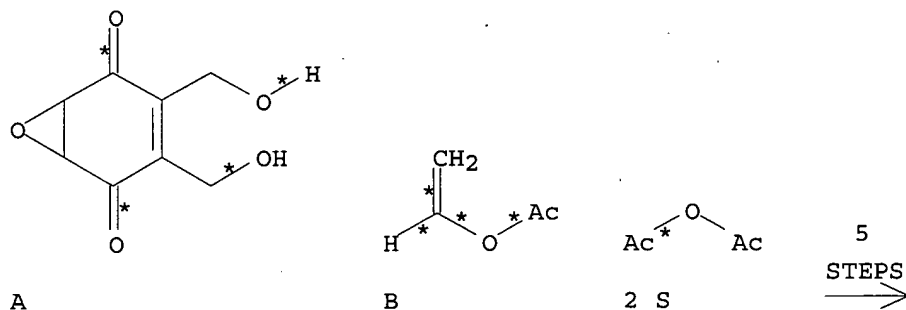
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH₄, J 7790-86-5 CeCl₃
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me₄-piperidoxyl, P 7782-44-7 O₂, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
PRO T 735317-28-9
SOL 75-09-2 CH₂Cl₂

RX(66) OF 87 COMPOSED OF RX(1), RX(2), RX(3), RX(5), RX(6)
RX(66) A + B + 2 S ==> T



T
YIELD 81%

Updated Search

10509228

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 109-99-9 THF
CON 0 deg C
NTE biotransformation, enzymic(lipase PS)

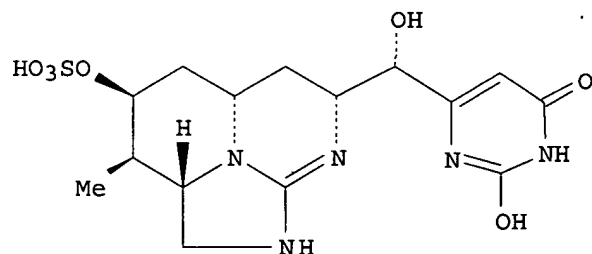
RX(2) RCT C 676263-74-4
RGT G 1191-15-7 AlH(Bu-i)2
PRO F 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(3) RCT F 676263-76-6
RGT I 16940-66-2 NaBH4, J 7790-86-5 CeCl3
PRO H 735317-25-6
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

RX(6) RCT N 735317-27-8, S 108-24-7
RGT U 110-86-1 Pyridine, V 1122-58-3 4-DMAP
PRO T 735317-28-9
SOL 75-09-2 CH2Cl2

L3 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 141:174352 CASREACT
TITLE: A concise asymmetric synthesis of the marine
hepatotoxin 7-epicyclindrospermopsin
AUTHOR(S): Looper, Ryan E.; Williams, Robert M.
CORPORATE SOURCE: Department of Chemistry, Colorado State University,
Fort Collins, CO, 80523, USA
SOURCE: Angewandte Chemie, International Edition (2004),
43(22), 2930-2933
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

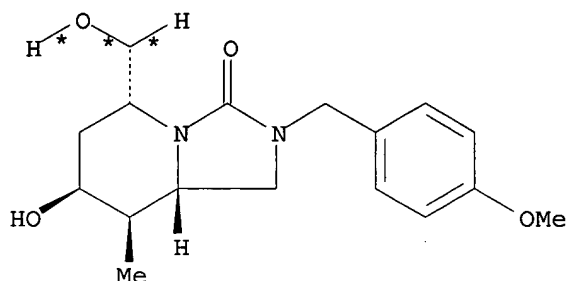
Updated Search

10509228

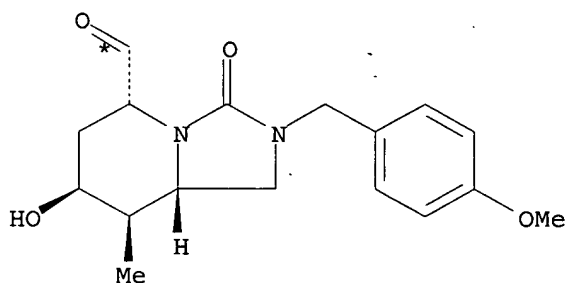
AB Born from a simple amino acid, the potent hepatotoxic cyanobacterial alkaloid 7-epicyclindrospermopsin (I) was synthesized through a concise asym. eighteen-step route. An intramol. 1,3-dipolar cycloaddn. and a nitroaldol reaction are key steps in the construction of the natural product from a precursor with a single stereogenic center.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 120 ...V ==> H...



V



H

YIELD 75%

RX(6) RCT V 732278-69-2
RGT W 3240-34-4 PhI(OAc)₂, X 2564-83-2 Me₄-piperidoxyl, Y
75-75-2 MeSO₃H
PRO H 732278-68-1
SOL 865-49-6 CDCl₃
CON 3 hours, room temperature

L3 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:54113 CASREACT

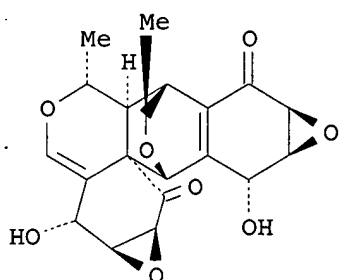
TITLE: Enantioselective total synthesis of (-)-epoxyquinols A and B. Novel, convenient access to chiral epoxyquinone building blocks through enzymatic desymmetrization

AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul

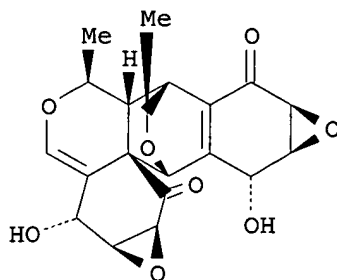
Updated Search

10509228

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India
SOURCE: Tetrahedron Letters (2004), 45(18), 3611-3615
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

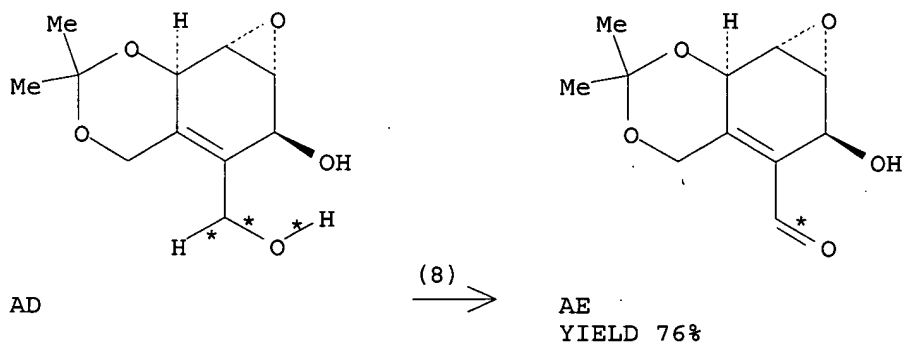


II

AB Following our recent total synthesis of the biol. potent natural products epoxyquinols A and B in racemic form, we have now accomplished the total synthesis of the (-)-epoxyquinols A (I) and B (II), antipodes of the angiogenesis inhibiting natural products, through a protocol that involves enzymic desymmetrization of a versatile epoxyquinone derivative, readily available from the Diels-Alder adduct of cyclopentadiene and p-benzoquinone.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(8) OF 307 ...AD ==> AE...

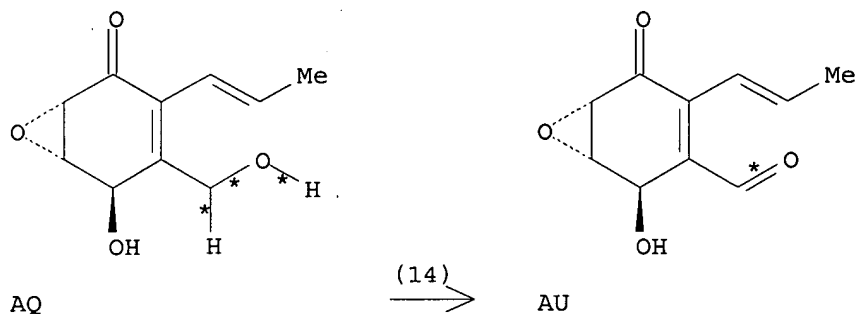


RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(14) OF 307 ...AQ ==> AU...

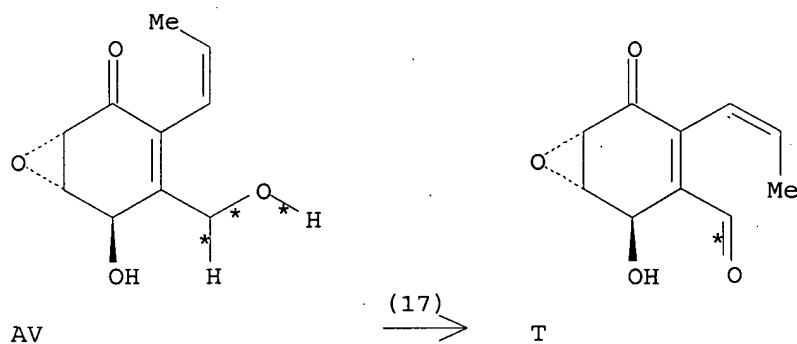
Updated Search

10509228



RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

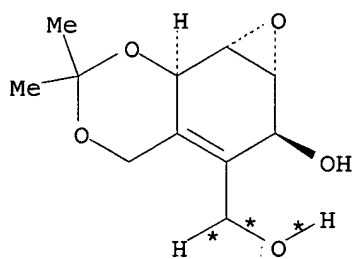
RX(17) OF 307 ...AV ==> T...



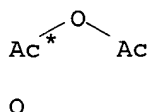
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(31) OF 307 COMPOSED OF RX(8), RX(9)
RX(31) AD + O ==> AJ

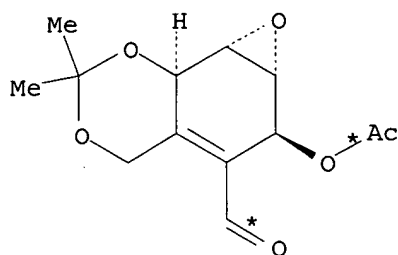
10509228



AD



2
STEPS
→



AJ

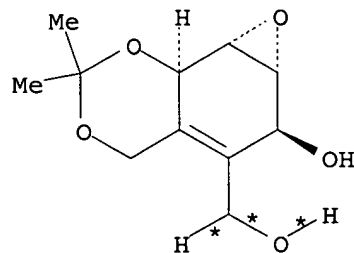
YIELD 87%

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

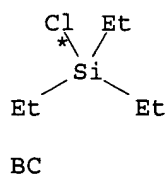
RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH2Cl2
CON 0 deg C

RX(32) OF 307 COMPOSED OF RX(8), RX(22)

RX(32) AD + BC ==> BD



AD

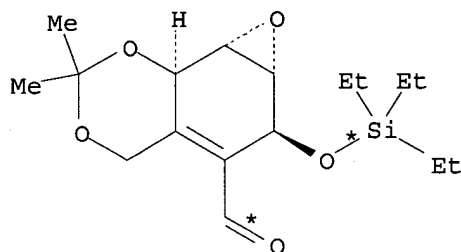


BC

2
STEPS
→

Updated Search

10509228

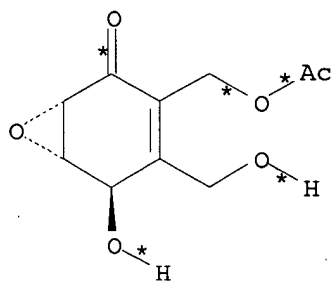


BD
YIELD 70%

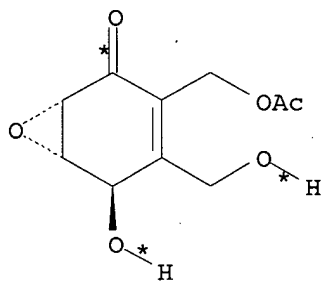
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

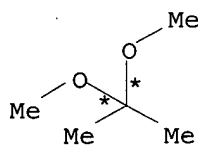
RX(57) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8)
RX(57) 2 L + 2 W ==> AE



L



L

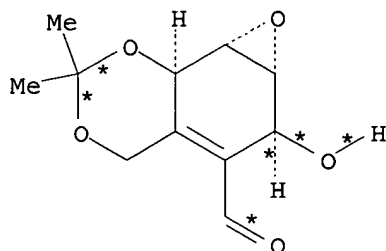


2 W

4
STEPS
→

Updated Search

10509228



AE

YIELD 76%

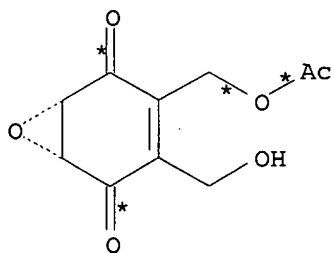
RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

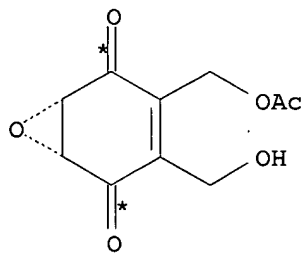
RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

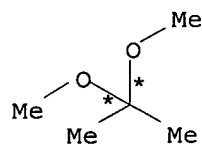
RX(109) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8)
RX(109) 2 C + 2 W ==> AE



C



C

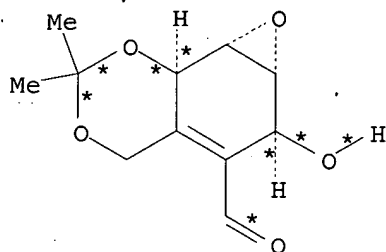


2 W

Updated Search

10509228

5
STEPS
→



AE
YIELD 76%

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

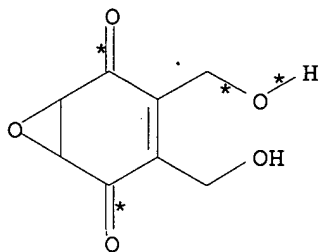
RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

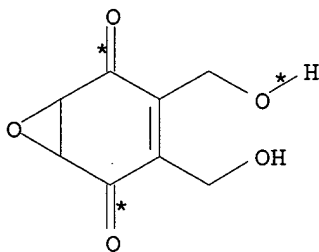
RX(110) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8)
RX(110) 2 A + 2 B + 2 W ==> AE

Updated Search

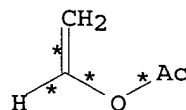
10509228



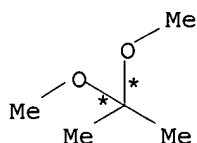
A



A

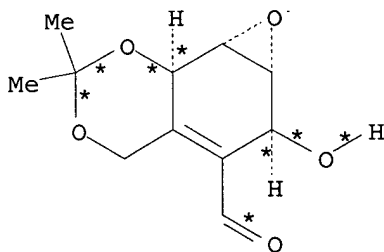


2 B



2 W

6
STEPS
→



AE

YIELD 76%

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

Updated Search

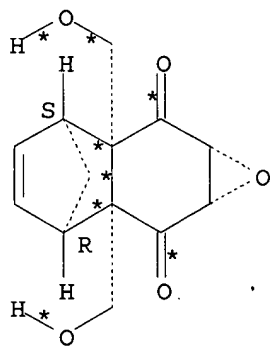
10509228

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

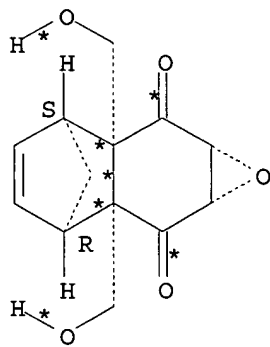
RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

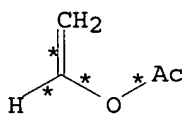
RX(111) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8)
RX(111) 2 AX + 2 B + 2 W ==> AE



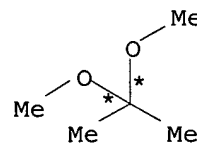
AX



AX



2 B

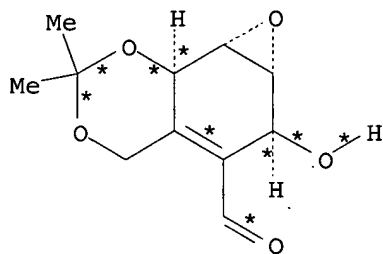


2 W

7
STEPS
→

Updated Search

10509228



AE

YIELD 76%

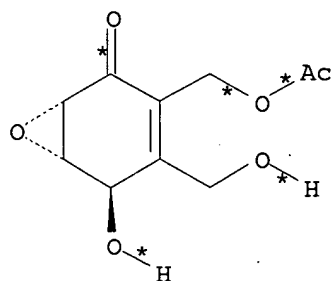
RX(19)	RCT	AX 556795-51-8
	PRO	A 556795-52-9
	SOL	101-84-8 PhOPh
	NTE	stereoselective
RX(1)	RCT	A 556795-52-9, B 108-05-4
	PRO	C 676263-74-4
	CAT	9001-62-1 Lipase
	SOL	1634-04-4 t-BuOMe
	CON	6 hours, 0 deg C
	NTE	biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
RX(3)	RCT	C 676263-74-4
	RGT	M 1191-15-7 AlH(Bu-i) ₂
	PRO	L 676263-76-6
	SOL	109-99-9 THF
	CON	-78 deg C
	NTE	stereoselective
RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me ₂ CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH ₄
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl ₃
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(21)	RCT	Z 701921-89-3
	RGT	AO 584-08-7 K ₂ CO ₃
	PRO	BB 701921-78-0, AD 701921-79-1
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(8)	RCT	AD 701921-79-1
	RGT	AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl

Updated Search

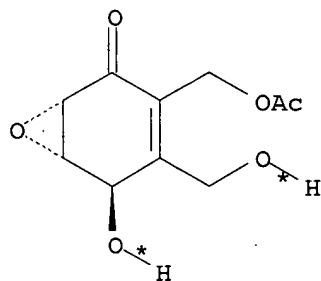
10509228

PRO AE 701921-80-4
SOL 68-12-2 DMF

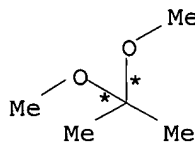
RX(113) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9)
RX(113) 2 L + 2 W + O ==> AJ



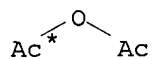
L



L

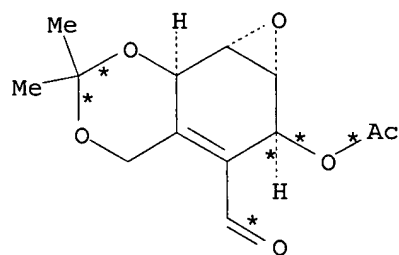


2 W



O

5
STEPS
→



AJ

YIELD 87%

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me2CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3

Updated Search

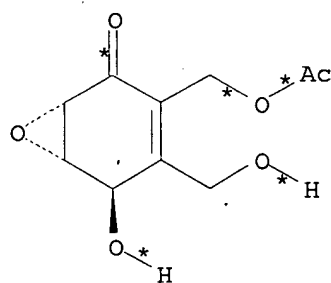
10509228

RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

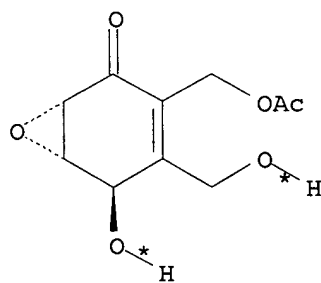
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

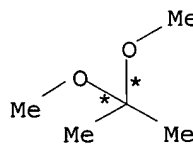
RX(114) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22)
RX(114) 2 L + 2 W + BC ==> BD



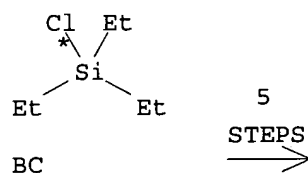
L



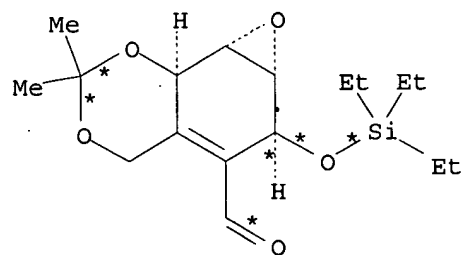
L



2 W



5
STEPS
→



BD
YIELD 70%

Updated Search

10509228

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me2CO
CON room temperature

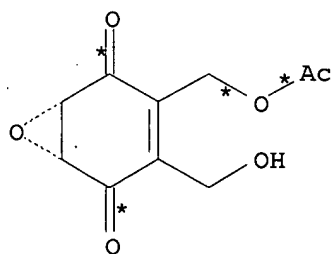
RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

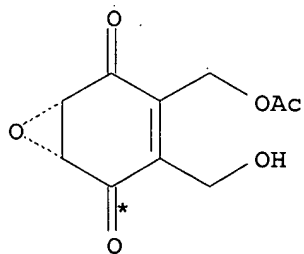
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH2Cl2
CON 0 deg C

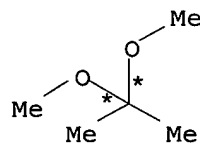
RX(115) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9)
RX(115) 2 C + 2 W + O ==> AJ



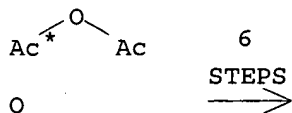
C



C

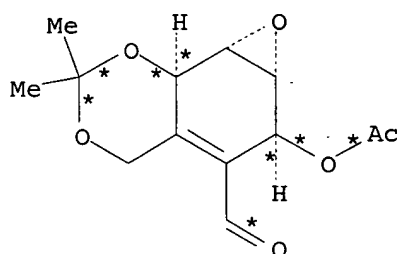


2 W



Updated Search

10509228



AJ
YIELD 87%

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

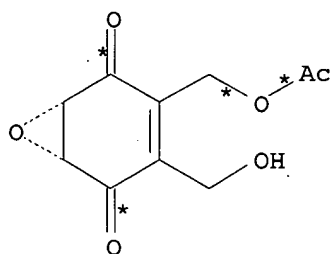
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

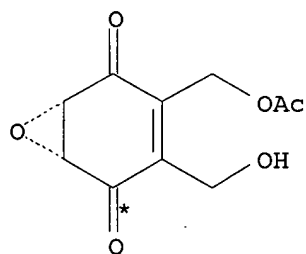
RX(116) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22)
RX(116) 2 C + 2 W + BC ==> BD

Updated Search

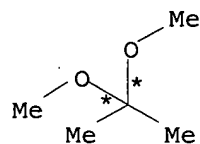
10509228



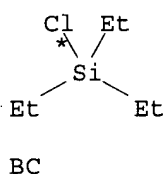
C



C

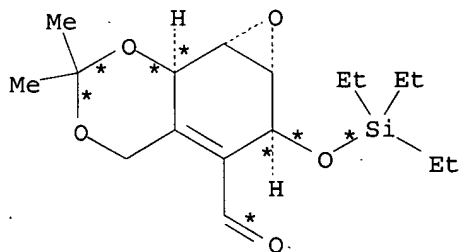


2 W



BC

6
STEPS
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BD

YIELD 70%

RX(3)	RCT	C 676263-74-4
	RGT	M 1191-15-7 AlH(Bu-i) ₂
	PRO	L 676263-76-6
	SOL	109-99-9 THF
	CON	-78 deg C
	NTE	stereoselective
RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me ₂ CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH ₄
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl ₃
	SOL	67-56-1 MeOH
	CON	0 deg C

Updated Search

10509228

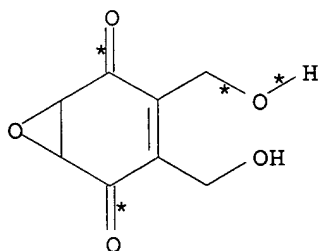
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

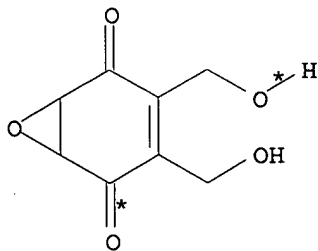
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH2Cl2
CON 0 deg C

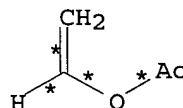
RX(117) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9)
RX(117) 2 A + 2 B + 2 W + O ==> AJ



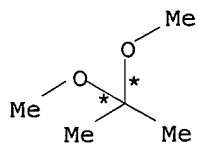
A



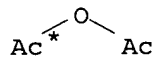
A



2 B



2 W

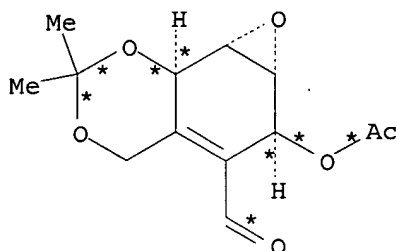


O

7
STEPS
→

Updated Search

10509228



AJ

YIELD 87%

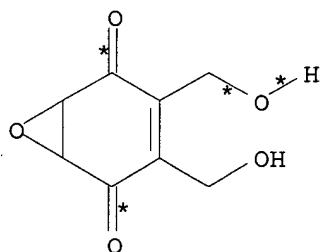
RX(1)	RCT A 556795-52-9, B 108-05-4
	PRO C 676263-74-4
	CAT 9001-62-1 Lipase
	SOL 1634-04-4 t-BuOMe
	CON 6 hours, 0 deg C
	NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
RX(3)	RCT C 676263-74-4
	RGT M 1191-15-7 AlH(Bu-i) ₂
	PRO L 676263-76-6
	SOL 109-99-9 THF
	CON -78 deg C
	NTE stereoselective
RX(6)	RCT L 676263-76-6, W 77-76-9
	RGT Y 24057-28-1 Pyridinium tosylate
	PRO X 701921-77-9
	SOL 67-64-1 Me ₂ CO
	CON room temperature
RX(7)	RCT X 701921-77-9
	RGT AA 16940-66-2 NaBH ₄
	PRO Z 701921-89-3
	CAT 7790-86-5 CeCl ₃
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(21)	RCT Z 701921-89-3
	RGT AO 584-08-7 K ₂ CO ₃
	PRO BB 701921-78-0, AD 701921-79-1
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(8)	RCT AD 701921-79-1
	RGT AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl
	PRO AE 701921-80-4
	SOL 68-12-2 DMF
RX(9)	RCT AE 701921-80-4, O 108-24-7
	RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP

Updated Search

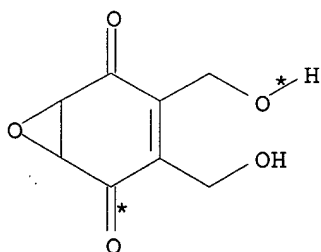
10509228

PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

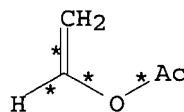
RX(118) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22)
RX(118) 2 A + 2 B + 2 W + BC ==> BD



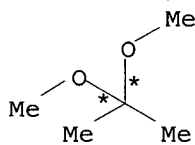
A



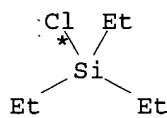
A



2 B

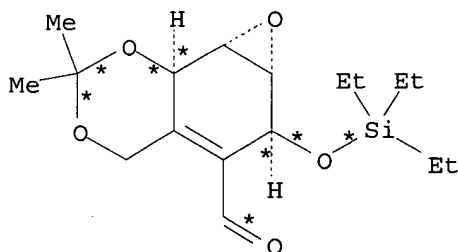


2 W



BC

7
STEPS
→



BD
YIELD 70%

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6

Updated Search

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SOL 109-99-9 THF
 CON -78 deg C
 NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
 RGT Y 24057-28-1 Pyridinium tosylate
 PRO X 701921-77-9
 SOL 67-64-1 Me2CO
 CON room temperature

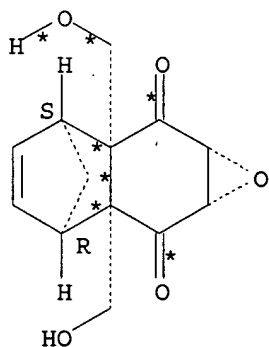
RX(7) RCT X 701921-77-9
 RGT AA 16940-66-2 NaBH4
 PRO Z 701921-89-3
 CAT 7790-86-5 CeCl3
 SOL 67-56-1 MeOH
 CON 0 deg C
 NTE stereoselective

RX(21) RCT Z 701921-89-3
 RGT AO 584-08-7 K2CO3
 PRO BB 701921-78-0, AD 701921-79-1
 SOL 67-56-1 MeOH
 CON 0 deg C
 NTE stereoselective

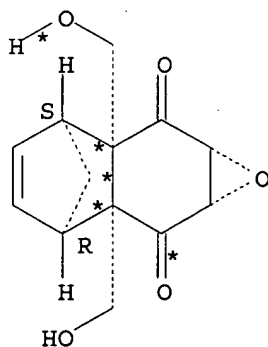
RX(8) RCT AD 701921-79-1
 RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
 Me4-piperidoxyl
 PRO AE 701921-80-4
 SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
 RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
 PRO BD 701921-90-6
 SOL 75-09-2 CH2Cl2
 CON 0 deg C

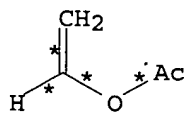
RX(119) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
 RX(9)
 RX(119) 2 AX + 2 B + 2 W + O ==> AJ



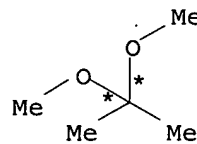
AX



AX



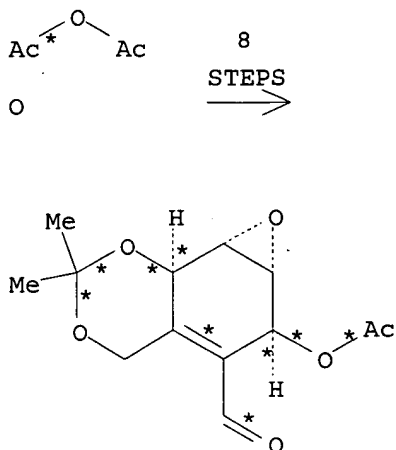
2 B



2 W

Updated Search

10509228



AJ

YIELD 87%

RX(19) RCT AX 556795-51-8
PRO A 556795-52-9
SOL 101-84-8 PhOPh
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)2
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me2CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1

Updated Search

10509228

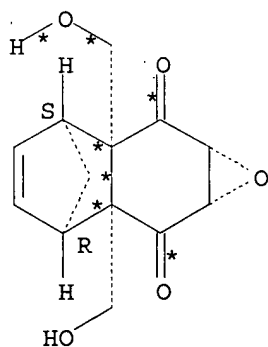
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

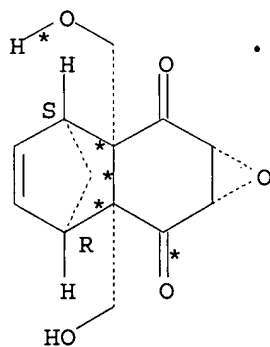
RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH2Cl2
CON 0 deg C

RX(120) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
RX(22)

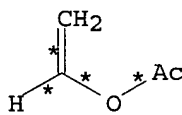
RX(120) 2 AX + 2 B + 2 W + BC ==> BD



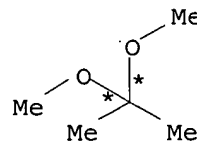
AX



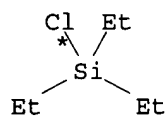
AX



2 B

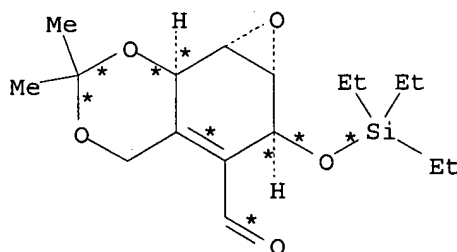


2 W



BC

8
STEPS
→



BD
YIELD 70%

RX(19) RCT AX 556795-51-8
PRO A 556795-52-9
SOL 101-84-8 PhOPh
NTE stereoselective

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RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)2
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me2CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

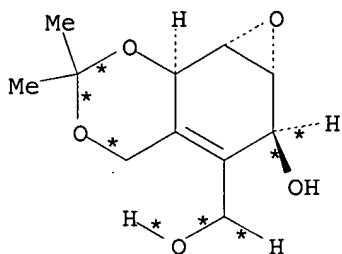
RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH2Cl2
CON 0 deg C

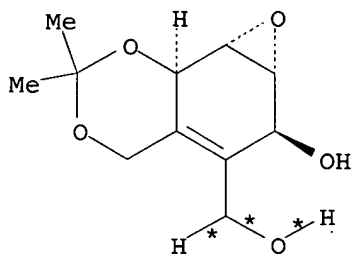
RX(155) OF 307 COMPOSED OF RX(8), RX(9), RX(10), RX(11), RX(13), RX(15), RX(17)
RX(155) 2 AD + 2 O + 2 AK ==> T

Updated Search

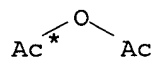
10509228



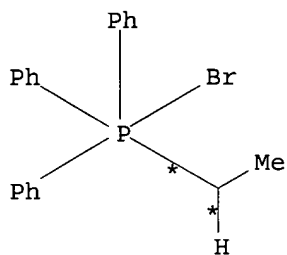
AD



AD

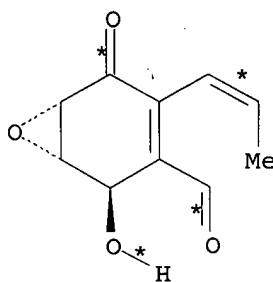


2 O



2 AK

7
STEPS
→



T

- RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF
- RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH2Cl2
CON 0 deg C
- RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective
- RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K2CO3
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C
- RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH2Cl2

Updated Search

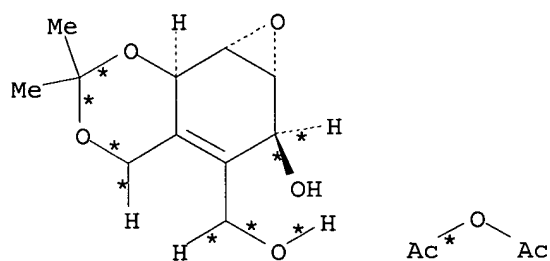
10509228

CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

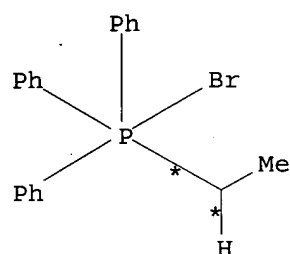
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(156) OF 307 COMPOSED OF RX(8), RX(9), RX(10), RX(11), RX(13), RX(12), RX(14)
RX(156) AD + O + AK ==> AU



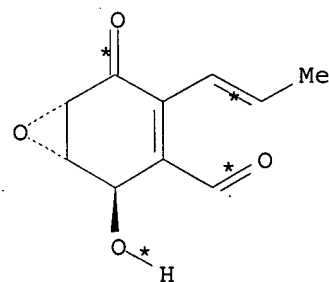
AD

O



AK

7
STEPS
→



AU

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5

Updated Search

10509228

SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

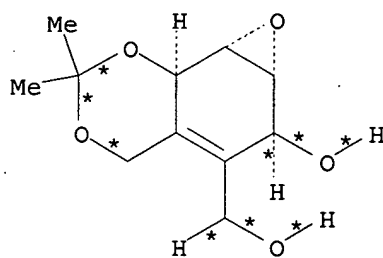
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

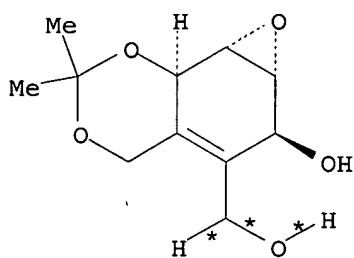
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(178) OF 307 COMPOSED OF RX(8), RX(22), RX(23), RX(24), RX(13), RX(15),
RX(17)

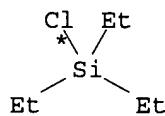
RX(178) 2 AD + BC + 2 AK ==> T



AD



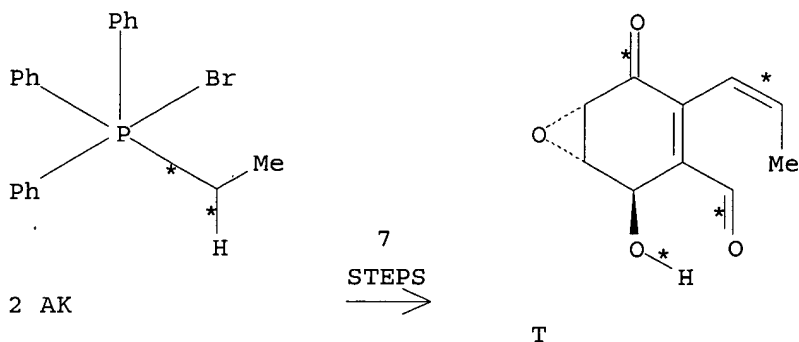
AD



BC

Updated Search

10509228



RX(8): RCT AD 701921-79-1
 RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
 Me₄-piperidoxyl
 PRO AE 701921-80-4
 SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
 RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
 PRO BD 701921-90-6
 SOL 75-09-2 CH₂Cl₂
 CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
 RGT AM 109-72-8 BuLi
 PRO BF 701921-91-7
 SOL 109-99-9 THF
 CON 0 deg C
 NTE stereoselective

RX(24) RCT BF 701921-91-7
 RGT BG 62778-11-4 Olah's reagent
 PRO AN 701921-92-8
 SOL 109-99-9 THF
 CON 0 deg C

RX(13) RCT AN 701921-92-8
 RGT AT 20039-37-6 PDC
 PRO AS 701921-84-8, AP 701921-83-7
 SOL 75-09-2 CH₂Cl₂
 CON 0 deg C
 NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
 RGT AR 9037-24-5 Amberlyst 15
 PRO AV 701921-85-9
 SOL 67-56-1 MeOH
 CON room temperature

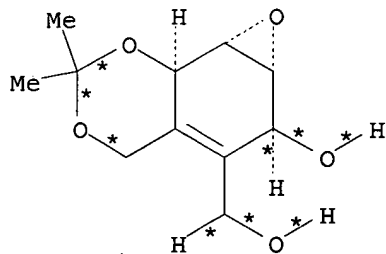
RX(17) RCT AV 701921-85-9
 RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
 Me₄-piperidoxyl
 PRO T 701921-87-1
 SOL 68-12-2 DMF
 CON room temperature

Updated Search

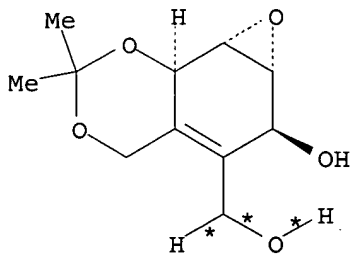
10509228

RX(179) OF 307 COMPOSED OF RX(8), RX(22), RX(23), RX(24), RX(13), RX(12),
RX(14)

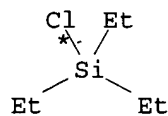
RX(179) 2 AD + BC + 2 AK ==> AU



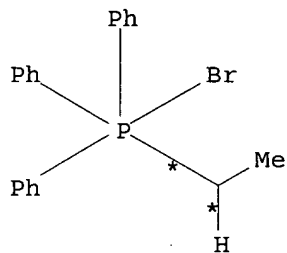
AD



AD

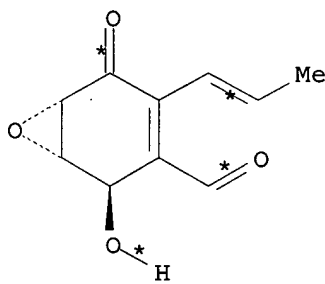


BC



2 AK

7
STEPS
→



AU

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF

Updated Search

10509228

CON 0 deg C

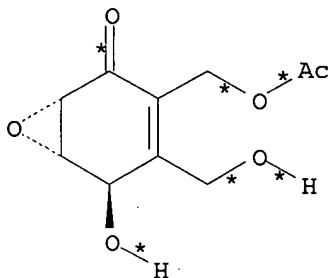
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH2Cl2
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

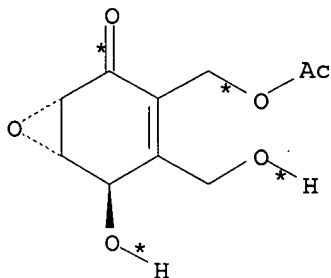
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(252) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9), RX(10), RX(11),
RX(13), RX(15), RX(17)

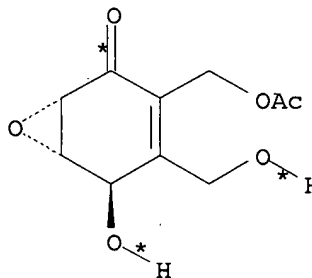
RX(252) 3 L + 3 W + 2 O + 2 AK ==> T



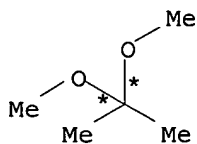
L



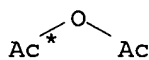
L



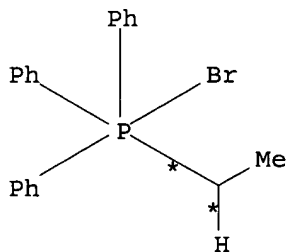
L



3 W



2 O

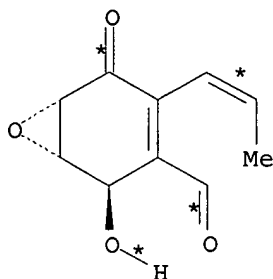


2 AK

10
STEPS
→

Updated Search

10509228



T

RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me2CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH4
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl3
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(21)	RCT	Z 701921-89-3
	RGT	AO 584-08-7 K2CO3
	PRO	BB 701921-78-0, AD 701921-79-1
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(8)	RCT	AD 701921-79-1
	RGT	AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
		Me4-piperidoxyl
	PRO	AE 701921-80-4
	SOL	68-12-2 DMF
RX(9)	RCT	AE 701921-80-4, O 108-24-7
	RGT	Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
	PRO	AJ 701921-81-5
	SOL	75-09-2 CH2Cl2
	CON	0 deg C
RX(10)	RCT	AJ 701921-81-5, AK 154489-89-1
	RGT	AM 109-72-8 BuLi
	PRO	AL 701921-82-6
	SOL	109-99-9 THF
	CON	0 deg C
	NTE	stereoselective
RX(11)	RCT	AL 701921-82-6
	RGT	AO 584-08-7 K2CO3
	PRO	AN 701921-92-8
	SOL	67-56-1 MeOH

Updated Search

10509228

CON 0 deg C

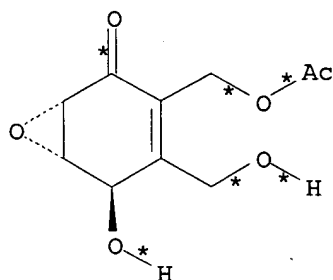
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

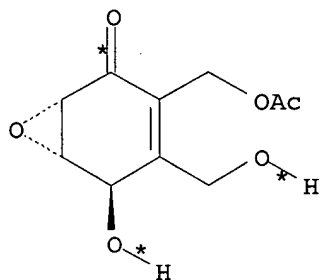
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(253) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(9), RX(10), RX(11),
RX(13), RX(12), RX(14)

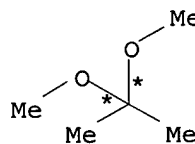
RX(253) 2 L + 2 W + O + AK ==> AU



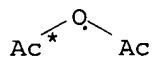
L



L



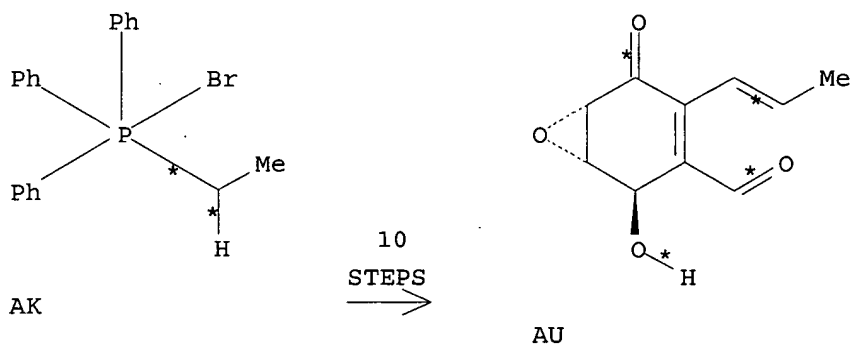
2 W



O

Updated Search

10509228



RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH

Updated Search

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CON 0 deg C

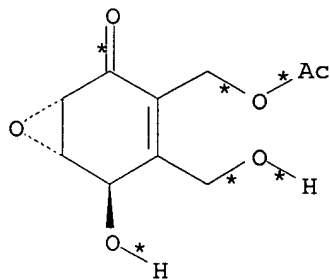
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

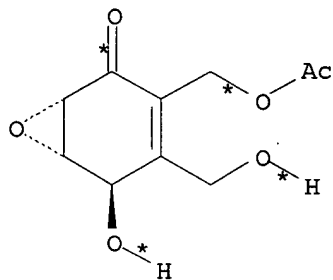
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(254) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22), RX(23), RX(24),
RX(13), RX(15), RX(17)

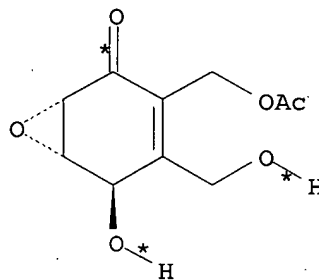
RX(254) 3 L + 3 W + 2 BC + 2 AK ==> T



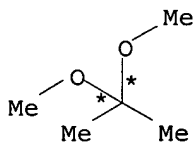
L



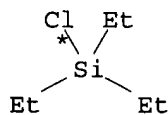
L



L



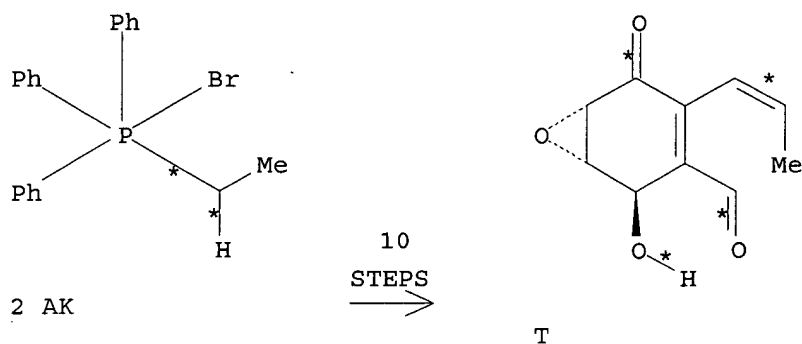
3 W



2 BC

Updated Search

10509228



- RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature
- RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective
- RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective
- RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF
- RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
- RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective
- RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF

Updated Search

10509228

CON 0 deg C

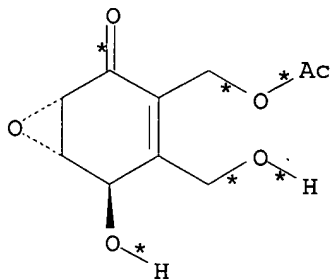
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

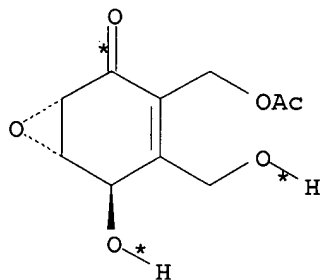
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(255) OF 307 COMPOSED OF RX(6), RX(7), RX(21), RX(8), RX(22), RX(23), RX(24),
RX(13), RX(12), RX(14)

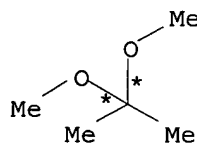
RX(255) 2 L + 2 W + BC + AK ==> AU



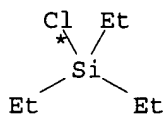
L



L



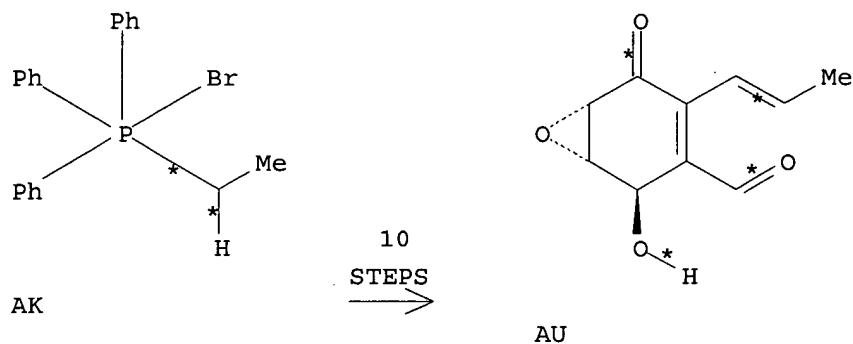
2 W



BC

Updated Search

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- RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature
- RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective
- RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective
- RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF
- RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
- RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective
- RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF

Updated Search

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CON 0 deg C

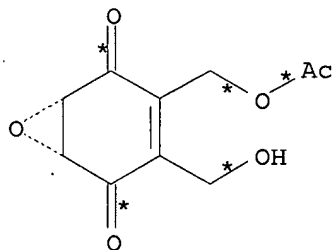
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

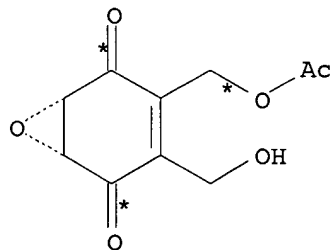
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(256) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9), RX(10),
RX(11), RX(13), RX(15), RX(17)

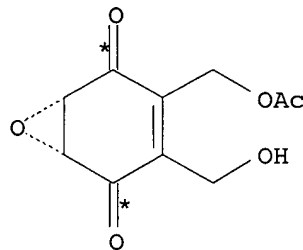
RX(256) 3 C + 3 W + 2 O + 2 AK ==> T



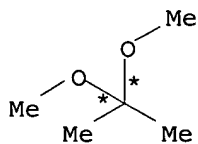
C



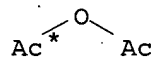
C



C



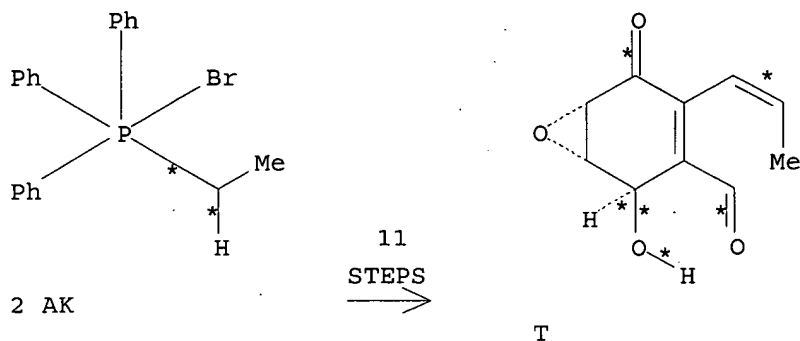
3 W



2 O

Updated Search

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RX(3)	RCT C 676263-74-4 RGT M 1191-15-7 AlH(Bu-i) ₂ PRO L 676263-76-6 SOL 109-99-9 THF CON -78 deg C NTE stereoselective
RX(6)	RCT L 676263-76-6, W 77-76-9 RGT Y 24057-28-1 Pyridinium tosylate PRO X 701921-77-9 SOL 67-64-1 Me ₂ CO CON room temperature
RX(7)	RCT X 701921-77-9 RGT AA 16940-66-2 NaBH ₄ PRO Z 701921-89-3 CAT 7790-86-5 CeCl ₃ SOL 67-56-1 MeOH CON 0 deg C NTE stereoselective
RX(21)	RCT Z 701921-89-3 RGT AO 584-08-7 K ₂ CO ₃ PRO BB 701921-78-0, AD 701921-79-1 SOL 67-56-1 MeOH CON 0 deg C NTE stereoselective
RX(8)	RCT AD 701921-79-1 RGT AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl PRO AE 701921-80-4 SOL 68-12-2 DMF
RX(9)	RCT AE 701921-80-4, O 108-24-7 RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP PRO AJ 701921-81-5 SOL 75-09-2 CH ₂ Cl ₂ CON 0 deg C
RX(10)	RCT AJ 701921-81-5, AK 154489-89-1 RGT AM 109-72-8 BuLi PRO AL 701921-82-6 SOL 109-99-9 THF

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CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

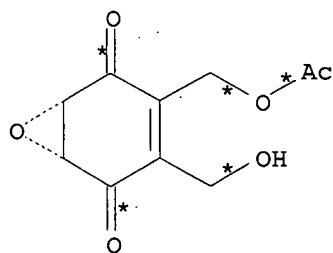
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

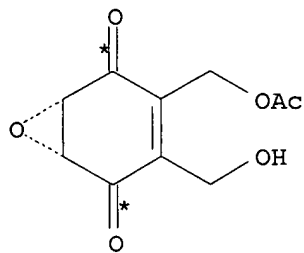
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(257) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(9), RX(10),
RX(11), RX(13), RX(12), RX(14)

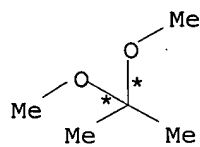
RX(257) 2 C + 2 W + O + AK ==> AU



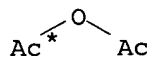
C



C



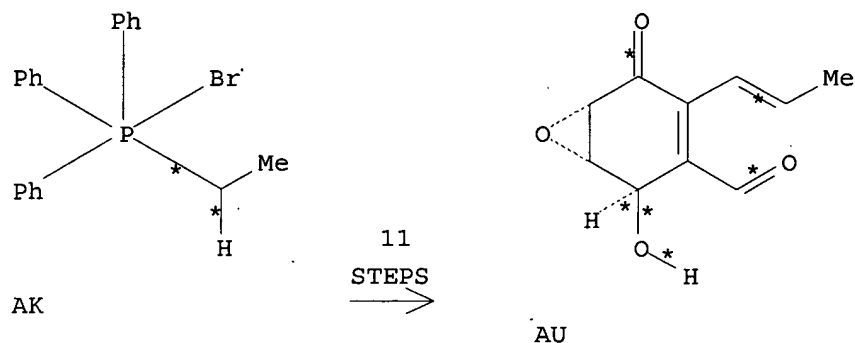
2 W



O

Updated Search

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RX(3)	RCT C 676263-74-4
	RGT M 1191-15-7 AlH(Bu-i) ₂
	PRO L 676263-76-6
	SOL 109-99-9 THF
	CON -78 deg C
	NTE stereoselective
RX(6)	RCT L 676263-76-6, W 77-76-9
	RGT Y 24057-28-1 Pyridinium tosylate
	PRO X 701921-77-9
	SOL 67-64-1 Me ₂ CO
	CON room temperature
RX(7)	RCT X 701921-77-9
	RGT AA 16940-66-2 NaBH ₄
	PRO Z 701921-89-3
	CAT 7790-86-5 CeCl ₃
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(21)	RCT Z 701921-89-3
	RGT AO 584-08-7 K ₂ CO ₃
	PRO BB 701921-78-0, AD 701921-79-1
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(8)	RCT AD 701921-79-1
	RGT AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl
	PRO AE 701921-80-4
	SOL 68-12-2 DMF
RX(9)	RCT AE 701921-80-4, O 108-24-7
	RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
	PRO AJ 701921-81-5
	SOL 75-09-2 CH ₂ Cl ₂
	CON 0 deg C
RX(10)	RCT AJ 701921-81-5, AK 154489-89-1
	RGT AM 109-72-8 BuLi
	PRO AL 701921-82-6
	SOL 109-99-9 THF

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CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

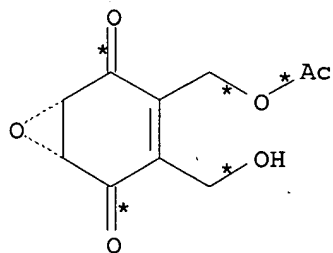
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

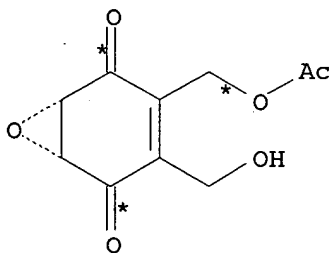
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(258) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22), RX(23),
RX(24), RX(13), RX(15), RX(17)

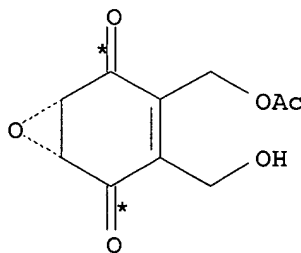
RX(258) 3 C + 3 W + 2 BC + 2 AK ==> T



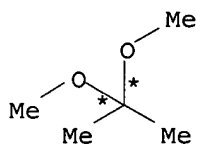
C



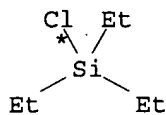
C



C



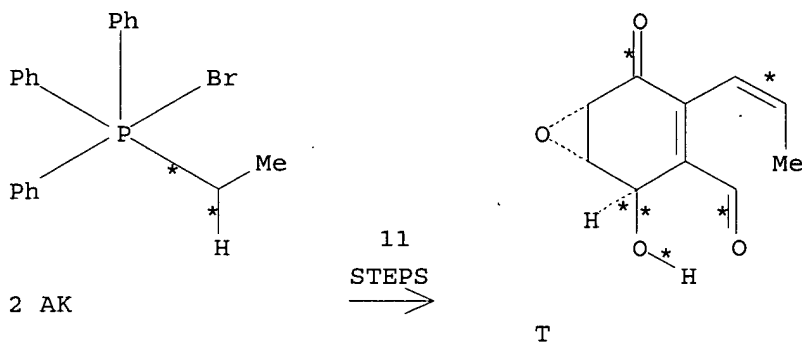
3 W



2 BC

Updated Search

10509228



RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF

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CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

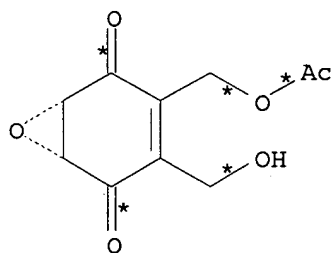
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

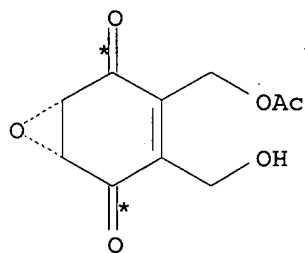
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(259) OF 307 COMPOSED OF RX(3), RX(6), RX(7), RX(21), RX(8), RX(22), RX(23),
RX(24), RX(13), RX(12), RX(14)

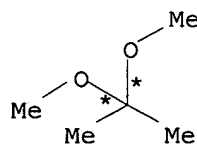
RX(259) 2 C + 2 W + BC + AK ==> AU



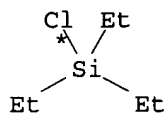
C



C



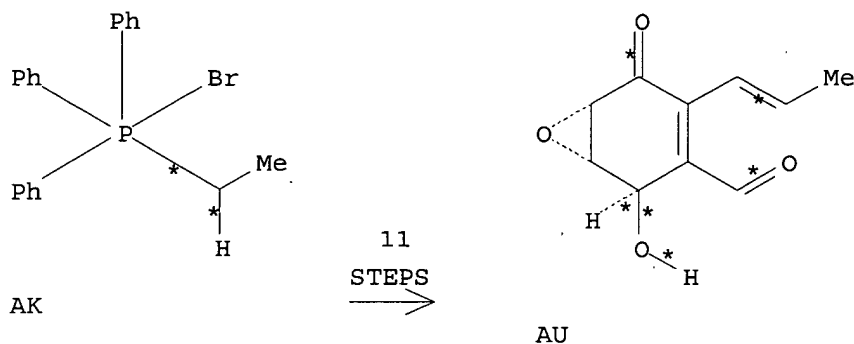
2 W



BC

Updated Search

10509228



RX(3)	RCT C 676263-74-4
	RGT M 1191-15-7 AlH(Bu-i) ₂
	PRO L 676263-76-6
	SOL 109-99-9 THF
	CON -78 deg C
	NTE stereoselective
RX(6)	RCT L 676263-76-6, W 77-76-9
	RGT Y 24057-28-1 Pyridinium tosylate
	PRO X 701921-77-9
	SOL 67-64-1 Me ₂ CO
	CON room temperature
RX(7)	RCT X 701921-77-9
	RGT AA 16940-66-2 NaBH ₄
	PRO Z 701921-89-3
	CAT 7790-86-5 CeCl ₃
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(21)	RCT Z 701921-89-3
	RGT AO 584-08-7 K ₂ CO ₃
	PRO BB 701921-78-0, AD 701921-79-1
	SOL 67-56-1 MeOH
	CON 0 deg C
	NTE stereoselective
RX(8)	RCT AD 701921-79-1
	RGT AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl
	PRO AE 701921-80-4
	SOL 68-12-2 DMF
RX(22)	RCT AE 701921-80-4, BC 994-30-9
	RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
	PRO BD 701921-90-6
	SOL 75-09-2 CH ₂ Cl ₂
	CON 0 deg C
RX(23)	RCT BD 701921-90-6, AK 154489-89-1
	RGT AM 109-72-8 BuLi
	PRO BF 701921-91-7
	SOL 109-99-9 THF

Updated Search

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CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

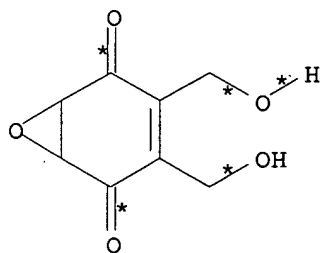
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

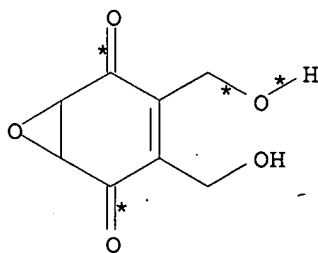
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(260) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9),
RX(10), RX(11), RX(13), RX(15), RX(17)

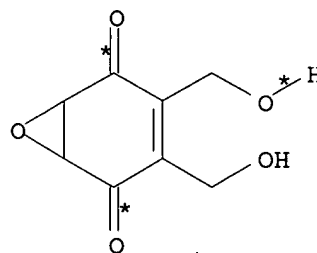
RX(260) 3 A + 3 B + 3 W + 2 O + 2 AK ==> T



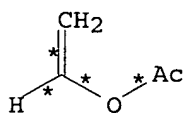
A



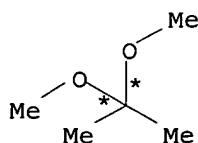
A



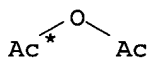
A



3 B



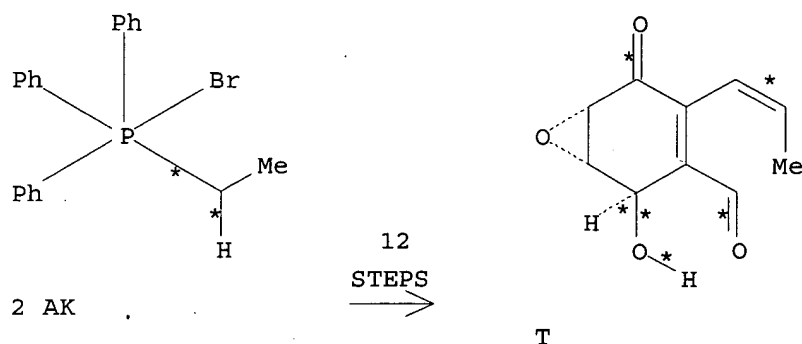
3 W



2 O

Updated Search

10509228



RX(1) RCT A 556795-52-9, B 108-05-4
 PRO C 676263-74-4
 CAT 9001-62-1 Lipase
 SOL 1634-04-4 t-BuOMe
 CON 6 hours, 0 deg C
 NTE biotransformation, enzymic, lipase PS 30(amino) used, stereoselective

RX(3) RCT C 676263-74-4
 RGT M 1191-15-7 AlH(Bu-i)₂
 PRO L 676263-76-6
 SOL 109-99-9 THF
 CON -78 deg C
 NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
 RGT Y 24057-28-1 Pyridinium tosylate
 PRO X 701921-77-9
 SOL 67-64-1 Me₂CO
 CON room temperature

RX(7) RCT X 701921-77-9
 RGT AA 16940-66-2 NaBH₄
 PRO Z 701921-89-3
 CAT 7790-86-5 CeCl₃
 SOL 67-56-1 MeOH
 CON 0 deg C
 NTE stereoselective

RX(21) RCT Z 701921-89-3
 RGT AO 584-08-7 K₂CO₃
 PRO BB 701921-78-0, AD 701921-79-1
 SOL 67-56-1 MeOH
 CON 0 deg C
 NTE stereoselective

RX(8) RCT AD 701921-79-1
 RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2 Me₄-piperidoxyl
 PRO AE 701921-80-4
 SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
 RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP

Updated Search

10509228

PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

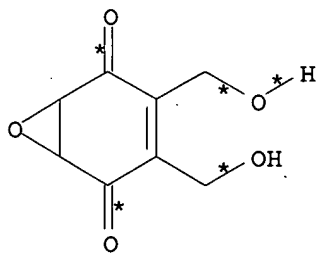
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

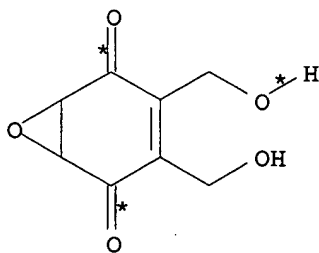
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(261) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(9),
RX(10), RX(11), RX(13), RX(12), RX(14)

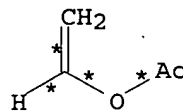
RX(261) 2 A + 2 B + 2 W + O + AK ==> AU



A

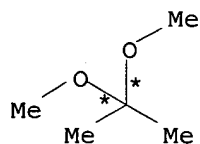


A

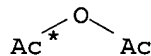


2 B

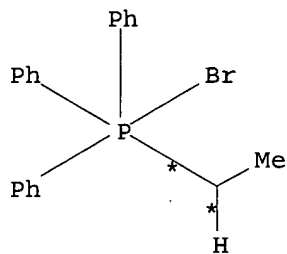
10509228



2 W

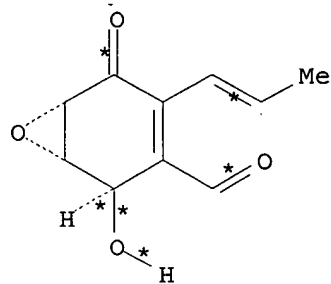


O



AK

12
STEPS
→



AU

- | | | |
|-------|-----|---|
| RX(1) | RCT | A 556795-52-9, B 108-05-4 |
| | PRO | C 676263-74-4 |
| | CAT | 9001-62-1 Lipase |
| | SOL | 1634-04-4 t-BuOMe |
| | CON | 6 hours, 0 deg C |
| | NTE | biotransformation, enzymic, lipase PS 30(amino) used, stereoselective |
| RX(3) | RCT | C 676263-74-4 |
| | RGT | M 1191-15-7 AlH(Bu-i) ₂ |
| | PRO | L 676263-76-6 |
| | SOL | 109-99-9 THF |
| | CON | -78 deg C |
| | NTE | stereoselective |
| RX(6) | RCT | L 676263-76-6, W 77-76-9 |
| | RGT | Y 24057-28-1 Pyridinium tosylate |
| | PRO | X 701921-77-9 |
| | SOL | 67-64-1 Me ₂ CO |
| | CON | room temperature |
| RX(7) | RCT | X 701921-77-9 |
| | RGT | AA 16940-66-2 NaBH ₄ |
| | PRO | Z 701921-89-3 |
| | CAT | 7790-86-5 CeCl ₃ |
| | SOL | 67-56-1 MeOH |
| | CON | 0 deg C |
| | NTE | stereoselective |

Updated Search

10509228

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

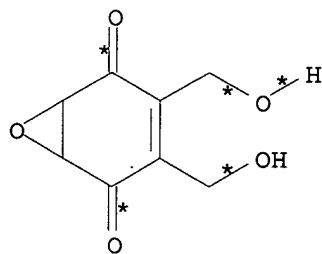
RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

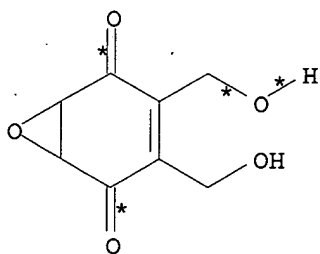
RX(262) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22),
RX(23), RX(24), RX(13), RX(15), RX(17)
RX(262) 3 A + 3 B + 3 W + 2 BC + 2 AK ==> T

Updated Search

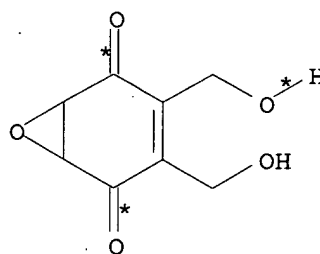
10509228



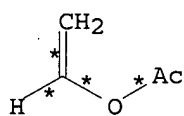
A



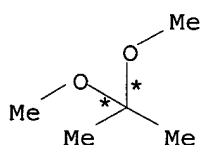
A



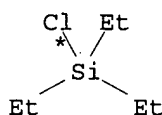
A



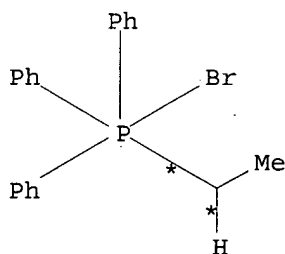
3 B



3 W

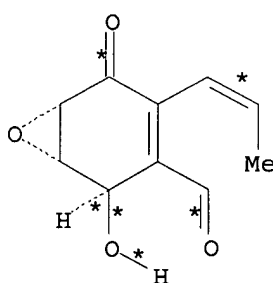


2 BC



2 AK

12
STEPS
→



T

RX(1)	RCT	A 556795-52-9, B 108-05-4
	PRO	C 676263-74-4
	CAT	9001-62-1 Lipase
	SOL	1634-04-4 t-BuOMe
	CON	6 hours, 0 deg C
	NTE	biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
RX(3)	RCT	C 676263-74-4
	RGT	M 1191-15-7 AlH(Bu-i)2
	PRO	L 676263-76-6
	SOL	109-99-9 THF
	CON	-78 deg C
	NTE	stereoselective
RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me2CO
	CON	room temperature

Updated Search

10509228

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

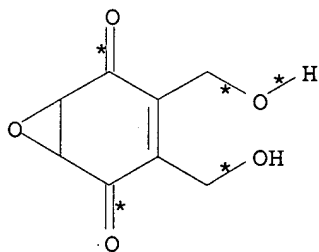
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF

Updated Search

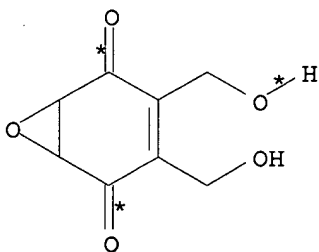
10509228

CON room temperature

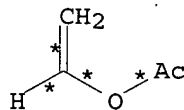
RX(263) OF 307 COMPOSED OF RX(1), RX(3), RX(6), RX(7), RX(21), RX(8), RX(22),
RX(23), RX(24), RX(13), RX(12), RX(14)
RX(263) 2 A + 2 B + 2 W + BC + AK ==> AU



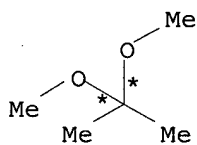
A



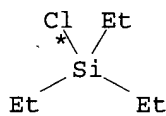
A



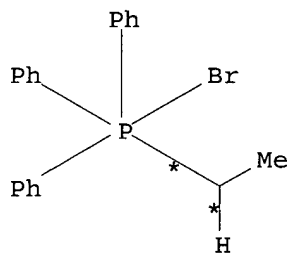
2 B



2 W

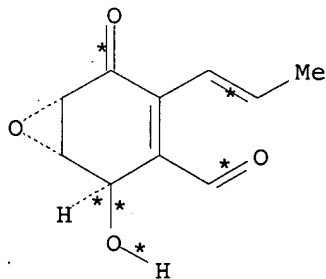


BC



AK

12
STEPS
→



AU

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

Updated Search

10509228

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

Updated Search

10509228

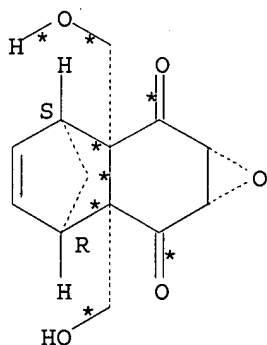
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

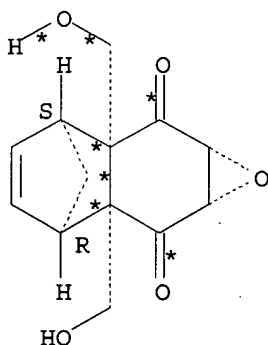
RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

RX(264) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
RX(9), RX(10), RX(11), RX(13), RX(15), RX(17)

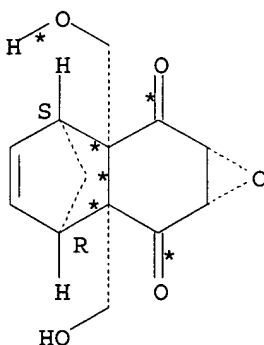
RX(264) 3 AX + 3 B + 3 W + 2 O + 2 AK ==> T



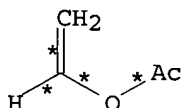
AX



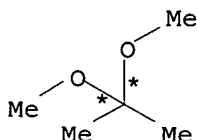
AX



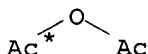
AX



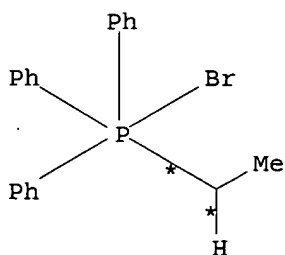
3 B



3 W

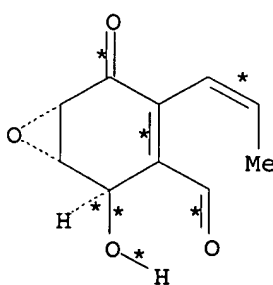


2 O



2 AK

13
STEPS
→



T

Updated Search

10509228

RX(19) RCT AX 556795-51-8
PRO A 556795-52-9
SOL 101-84-8 PhOPh
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C

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10509228

NTE stereoselective

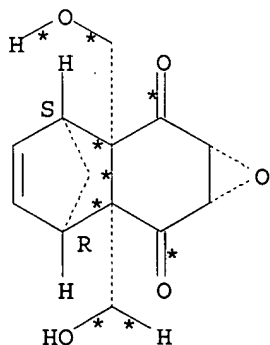
RX(11) RCT AL 701921-82-6
 RGT AO 584-08-7 K₂CO₃
 PRO AN 701921-92-8
 SOL 67-56-1 MeOH
 CON 0 deg C

RX(13) RCT AN 701921-92-8
 RGT AT 20039-37-6 PDC
 PRO AS 701921-84-8, AP 701921-83-7
 SOL 75-09-2 CH₂Cl₂
 CON 0 deg C
 NTE stereoselective, 81% overall yield

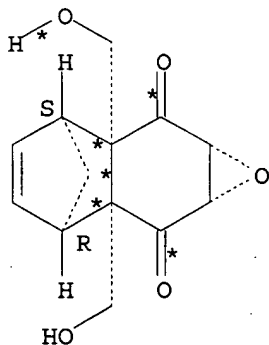
RX(15) RCT AS 701921-84-8
 RGT AR 9037-24-5 Amberlyst 15
 PRO AV 701921-85-9
 SOL 67-56-1 MeOH
 CON room temperature

RX(17) RCT AV 701921-85-9
 RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
 Me₄-piperidoxyl
 PRO T 701921-87-1
 SOL 68-12-2 DMF
 CON room temperature

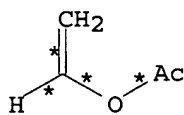
RX(265) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
 RX(9), RX(10), RX(11), RX(13), RX(12), RX(14)
 RX(265) 2 AX + 2 B + 2 W + O + AK ==> AU



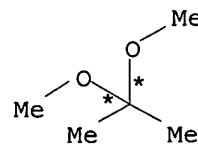
AX



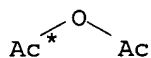
AX



2 B



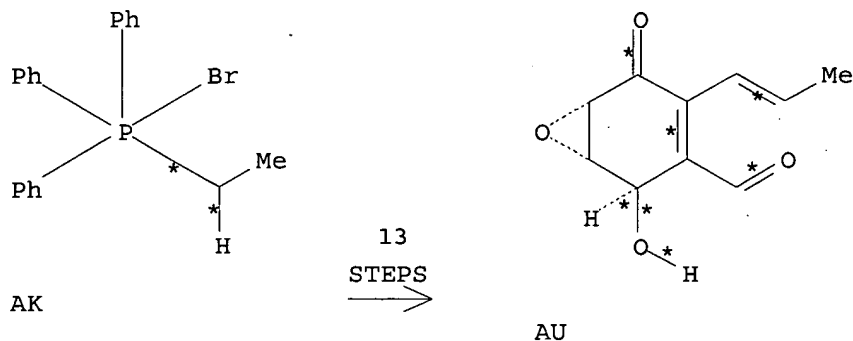
2 W



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10509228



RX(19)	RCT	AX 556795-51-8
	PRO	A 556795-52-9
	SOL	101-84-8 PhOPh
	NTE	stereoselective
RX(1)	RCT	A 556795-52-9, B 108-05-4
	PRO	C 676263-74-4
	CAT	9001-62-1 Lipase
	SOL	1634-04-4 t-BuOMe
	CON	6 hours, 0 deg C
	NTE	biotransformation, enzymic, lipase PS 30(amino) used, stereoselective
RX(3)	RCT	C 676263-74-4
	RGT	M 1191-15-7 AlH(Bu-i) ₂
	PRO	L 676263-76-6
	SOL	109-99-9 THF
	CON	-78 deg C
	NTE	stereoselective
RX(6)	RCT	L 676263-76-6, W 77-76-9
	RGT	Y 24057-28-1 Pyridinium tosylate
	PRO	X 701921-77-9
	SOL	67-64-1 Me ₂ CO
	CON	room temperature
RX(7)	RCT	X 701921-77-9
	RGT	AA 16940-66-2 NaBH ₄
	PRO	Z 701921-89-3
	CAT	7790-86-5 CeCl ₃
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(21)	RCT	Z 701921-89-3
	RGT	AO 584-08-7 K ₂ CO ₃
	PRO	BB 701921-78-0, AD 701921-79-1
	SOL	67-56-1 MeOH
	CON	0 deg C
	NTE	stereoselective
RX(8)	RCT	AD 701921-79-1
	RGT	AF 7782-44-7 O ₂ , AG 7758-89-6 CuCl, AH 2564-83-2 Me ₄ -piperidoxyl

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PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(9) RCT AE 701921-80-4, O 108-24-7
RGT Q 110-86-1 Pyridine, R 1122-58-3 4-DMAP
PRO AJ 701921-81-5
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(10) RCT AJ 701921-81-5, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO AL 701921-82-6
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(11) RCT AL 701921-82-6
RGT AO 584-08-7 K₂CO₃
PRO AN 701921-92-8
SOL 67-56-1 MeOH
CON 0 deg C

RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

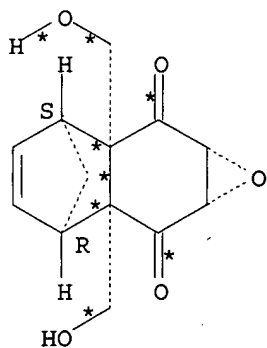
RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

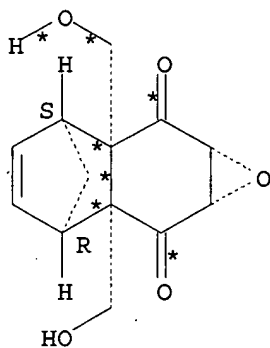
RX(266) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
RX(22), RX(23), RX(24), RX(13), RX(15), RX(17)

RX(266) 3 AX + 3 B + 3 W + 2 BC + 2 AK ==> T

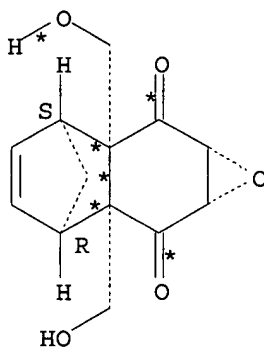
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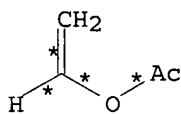
AX



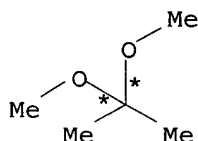
AX



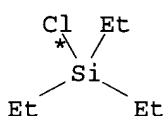
AX



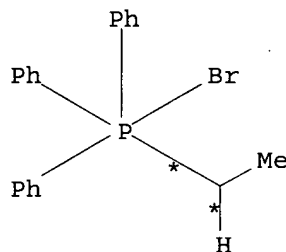
3 B



3 W

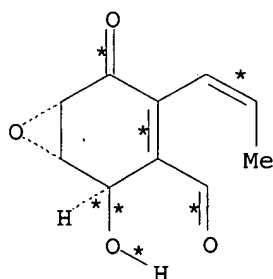


2 BC



2 AK

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STEPS
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RX(19) RCT AX 556795-51-8
PRO A 556795-52-9
SOL 101-84-8 PhOPh
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4

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PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)₂
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me₂CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH₄
PRO Z 701921-89-3
CAT 7790-86-5 CeCl₃
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K₂CO₃
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH₂Cl₂
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

Updated Search

10509228

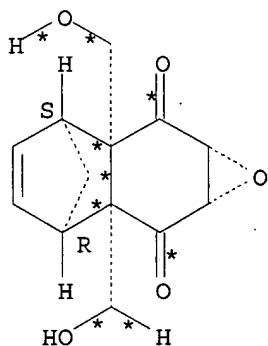
RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(15) RCT AS 701921-84-8
RGT AR 9037-24-5 Amberlyst 15
PRO AV 701921-85-9
SOL 67-56-1 MeOH
CON room temperature

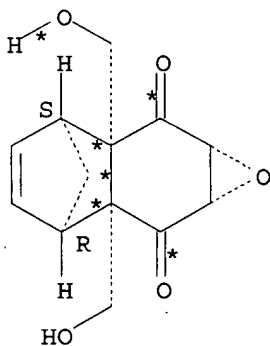
RX(17) RCT AV 701921-85-9
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO T 701921-87-1
SOL 68-12-2 DMF
CON room temperature

RX(267) OF 307 COMPOSED OF RX(19), RX(1), RX(3), RX(6), RX(7), RX(21), RX(8),
RX(22), RX(23), RX(24), RX(13), RX(12), RX(14)

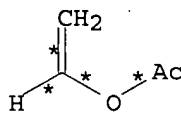
RX(267) 2 AX + 2 B + 2 W + BC + AK ==> AU



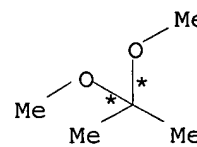
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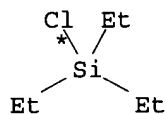
AX



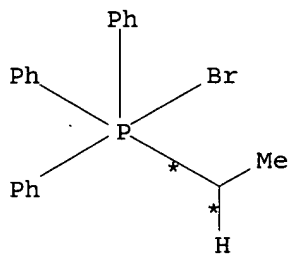
2 B



2 W

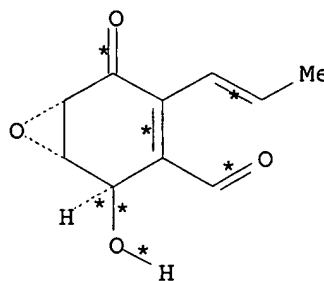


BC



AK

13
STEPS
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AU

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RX(19) RCT AX 556795-51-8
PRO A 556795-52-9
SOL 101-84-8 PhOPh
NTE stereoselective

RX(1) RCT A 556795-52-9, B 108-05-4
PRO C 676263-74-4
CAT 9001-62-1 Lipase
SOL 1634-04-4 t-BuOMe
CON 6 hours, 0 deg C
NTE biotransformation, enzymic, lipase PS 30(amino) used,
stereoselective

RX(3) RCT C 676263-74-4
RGT M 1191-15-7 AlH(Bu-i)2
PRO L 676263-76-6
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(6) RCT L 676263-76-6, W 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
PRO X 701921-77-9
SOL 67-64-1 Me2CO
CON room temperature

RX(7) RCT X 701921-77-9
RGT AA 16940-66-2 NaBH4
PRO Z 701921-89-3
CAT 7790-86-5 CeCl3
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(21) RCT Z 701921-89-3
RGT AO 584-08-7 K2CO3
PRO BB 701921-78-0, AD 701921-79-1
SOL 67-56-1 MeOH
CON 0 deg C
NTE stereoselective

RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O2, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

RX(22) RCT AE 701921-80-4, BC 994-30-9
RGT BE 288-32-4 1H-Imidazole, R 1122-58-3 4-DMAP
PRO BD 701921-90-6
SOL 75-09-2 CH2Cl2
CON 0 deg C

RX(23) RCT BD 701921-90-6, AK 154489-89-1
RGT AM 109-72-8 BuLi
PRO BF 701921-91-7
SOL 109-99-9 THF
CON 0 deg C
NTE stereoselective

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RX(24) RCT BF 701921-91-7
RGT BG 62778-11-4 Olah's reagent
PRO AN 701921-92-8
SOL 109-99-9 THF
CON 0 deg C

RX(13) RCT AN 701921-92-8
RGT AT 20039-37-6 PDC
PRO AS 701921-84-8, AP 701921-83-7
SOL 75-09-2 CH₂Cl₂
CON 0 deg C
NTE stereoselective, 81% overall yield

RX(12) RCT AP 701921-83-7
RGT AR 9037-24-5 Amberlyst 15
PRO AQ 494196-00-8
SOL 67-56-1 MeOH
CON room temperature

RX(14) RCT AQ 494196-00-8
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me₄-piperidoxyl
PRO AU 701921-86-0
SOL 68-12-2 DMF
CON room temperature

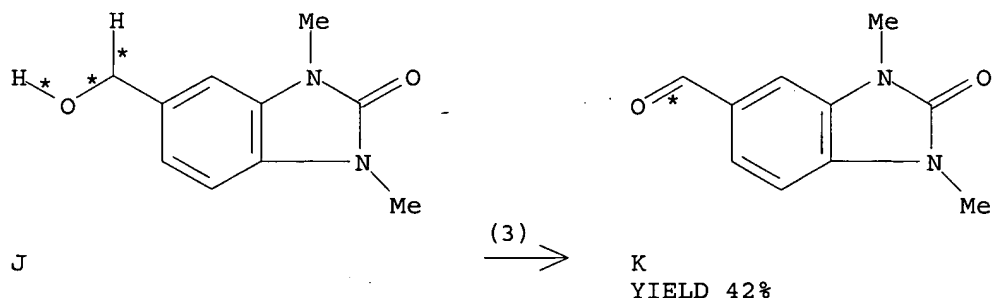
L3 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:339244 CASREACT
TITLE: Benzimidazolone p38 inhibitors
AUTHOR(S): Dombroski, Mark A.; Letavic, Michael A.; McClure, Kim
F.; Barberia, John T.; Carty, Thomas J.; Cortina,
Santo R.; Csiki, Csilla; Dipesa, Alan J.; Elliott,
Nancy C.; Gabel, Christopher A.; Jordan, Crystal K.;
Labasi, Jeff M.; Martin, William H.; Peese, Kevin M.;
Stock, Ingrid A.; Svensson, Linne; Sweeney, Francis
J.; Yu, Chul H.
CORPORATE SOURCE: Pfizer Global Research and Development, Groton
Laboratories, Groton, CT, 06340, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),
14(4), 919-923
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and in vitro p38 α activity of a novel series of
benzimidazolone inhibitors is described. The p38 α SAR is consistent
with a mode of binding wherein the benzimidazolone carbonyl serves as the
H-bond acceptor to Met109 of p38 α in a manner analogous to the
pyridine nitrogen of prototypical pyridylimidazole p38 inhibitors. Potent
p38 α activity comparable to that of several previously reported p38
inhibitors is observed for this novel chemotype.
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 443 ...J ==> K...

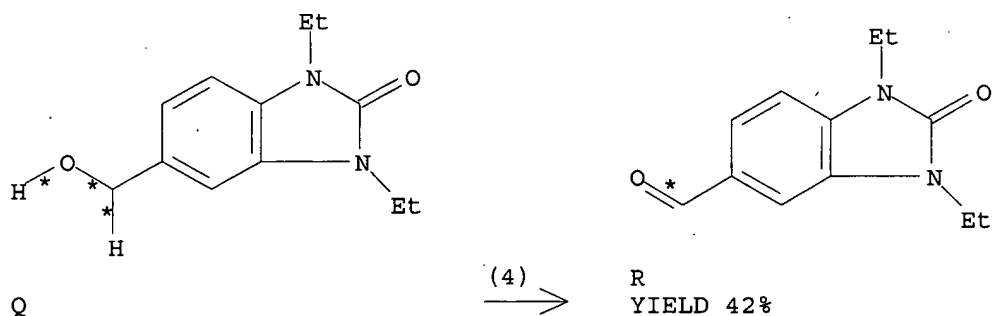
Updated Search

10509228



RX(3) RCT J 345657-96-7
RGT L 2564-83-2 Me4-piperidoxyl, M 128-09-6
Chlorosuccinimide
PRO K 55241-49-1
CAT 1112-67-0 Bu4NCl
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 5.5 hours, room temperature, pH 8.6
NTE buffered soln.

RX(4) OF 443 ...Q ==> R...



RX(4) RCT Q 864512-93-6
RGT L 2564-83-2 Me4-piperidoxyl, M 128-09-6
Chlorosuccinimide
PRO R 14624-85-2
CAT 1112-67-0 Bu4NCl
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 5.5 hours, room temperature, pH 8.6
NTE buffered soln.

L3 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:321153 CASREACT
TITLE: Enantioselective total synthesis of
(+)-panepophenanthrin, a novel inhibitor of the
ubiquitin-activating enzyme
AUTHOR(S): Mehta, Goverdhan; Ramesh, Senaiar S.
CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of
Science, Bangalore, 560 012, India
SOURCE: Tetrahedron Letters (2004), 45(9), 1985-1987

Updated Search

10509228

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
GI

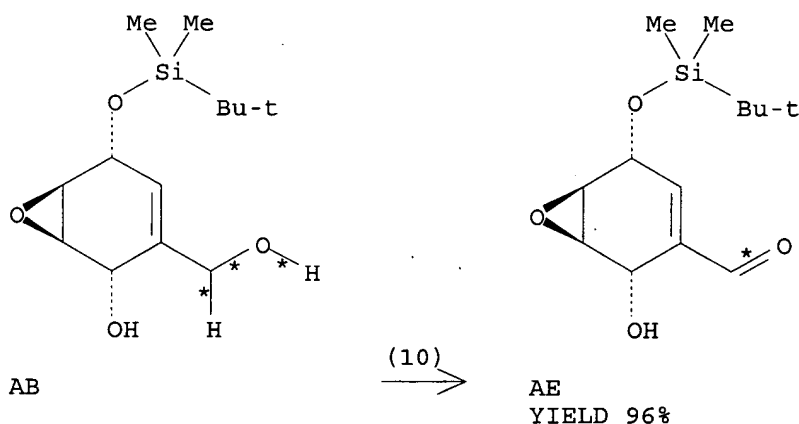
CODEN: TELEAY; ISSN: 0040-4039
Elsevier Science B.V.
Journal
English

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB An enantioselective total synthesis of the novel natural product (+)-panepophenanthrin (I) has been accomplished in which a biomimetic Diels-Alder dimerization is a key step. The monomeric precursor II was assembled from the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone through a short, simple sequence employing chemo- and stereoselective operations.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(10) OF 115 ...AB ==> AE...

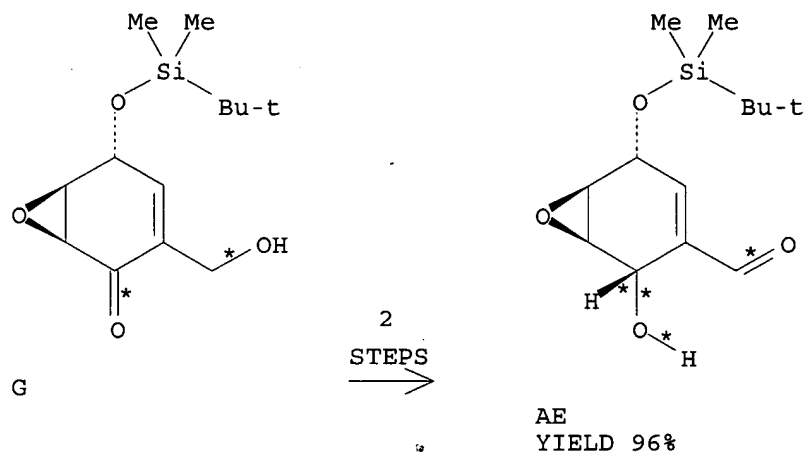


RX(10) RCT AB 678197-28-9
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH
7758-89-6 CuCl
PRO AE 678197-29-0
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

RX(23) OF 115 COMPOSED OF RX(9), RX(10)
RX(23) G ==> AE

Updated Search

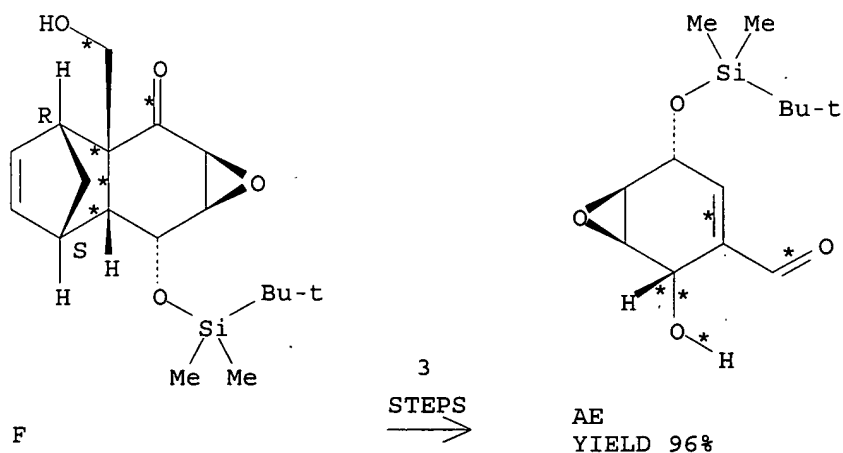
10509228



RX(9) RCT G 678197-25-6
RGT AC 1191-15-7 AlH(Bu-i)₂
PRO AB 678197-28-9
SOL 109-99-9 THF, 110-54-3 Hexane
CON 10 minutes, -78 deg C
NTE stereoselective

RX(10) RCT AB 678197-28-9
RGT AF 2564-83-2 Me₄-piperidoxyl, AG 7782-44-7 O₂, AH
7758-89-6 CuCl
PRO AE 678197-29-0
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

RX(30) OF 115 COMPOSED OF RX(3), RX(9), RX(10)
RX(30) F ==> AE



RX(3) RCT F 678197-27-8
PRO G 678197-25-6

Updated Search

10509228

SOL 101-84-8 PhOPh
CON 240 deg C

RX(9) RCT G 678197-25-6
RGT AC 1191-15-7 AlH(Bu-i)2
PRO AB 678197-28-9
SOL 109-99-9 THF, 110-54-3 Hexane
CON 10 minutes, -78 deg C
NTE stereoselective

RX(10) RCT AB 678197-28-9
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH
7758-89-6 CuCl
PRO AE 678197-29-0
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

L3 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:287206 CASREACT

TITLE: Total Synthesis of the Novel NF- κ B Inhibitor
(-)-Cycloepoxydon

AUTHOR(S): Mehta, Goverdhan; Islam, Kabirul

CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of
Science, Bangalore, 560 012, India

SOURCE: Organic Letters (2004), 6(5), 807-810

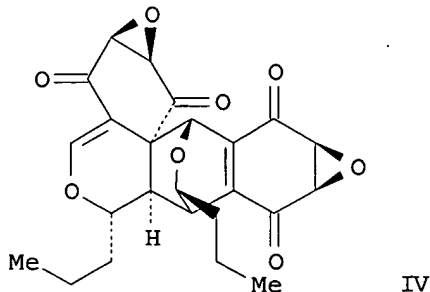
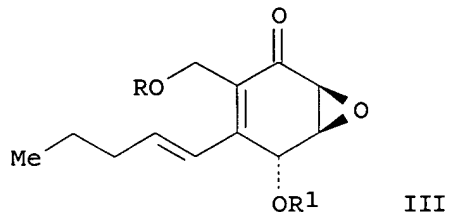
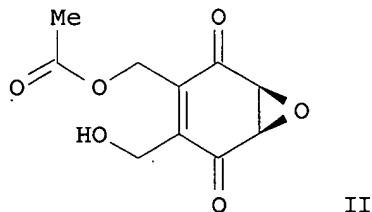
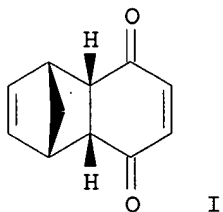
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB An enantioselective total synthesis of the novel, biol. active
epoxyquinone natural product (-)-cycloepoxydon has been accomplished from

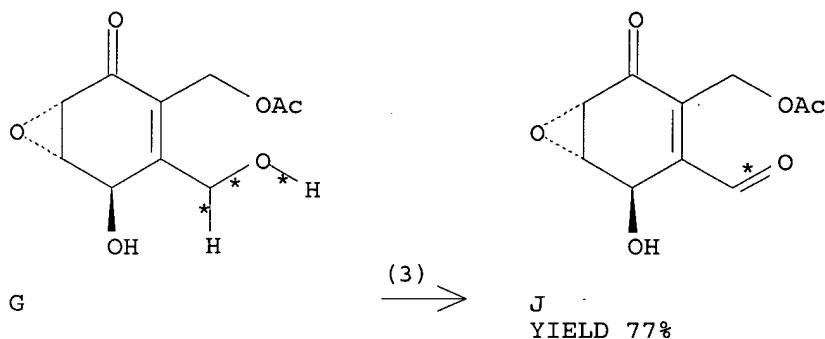
Updated Search

10509228

the readily available Diels-Alder adduct of cyclopentadiene and p-benzoquinone I. Epoxyquinone II, derived from I, was transformed into pentenyl epoxy acetate III (R = R1 = COMe), which was hydrolyzed and protected to give III (R = SiMe2CMe3, R1 = H). The latter compound underwent epoxidn. of the linear chain alkene and deprotection to give the title compound. A new cycloepoxydon related heptacyclic dimer IV has also been prepared from III (R = SiMe2CMe3, R1 = H) and characterized.

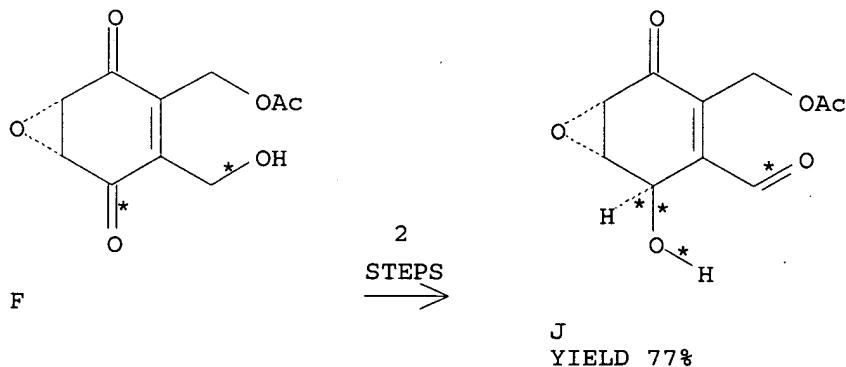
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 100 ...G ==> J...



RX(3) RCT G 676263-76-6
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2
PRO J 676263-78-8
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

RX(13) OF 100 COMPOSED OF RX(2), RX(3)
RX(13) F ==> J



RX(2) RCT F 676263-74-4
RGT H 1191-15-7 AlH(Bu-i)2
PRO G 676263-76-6

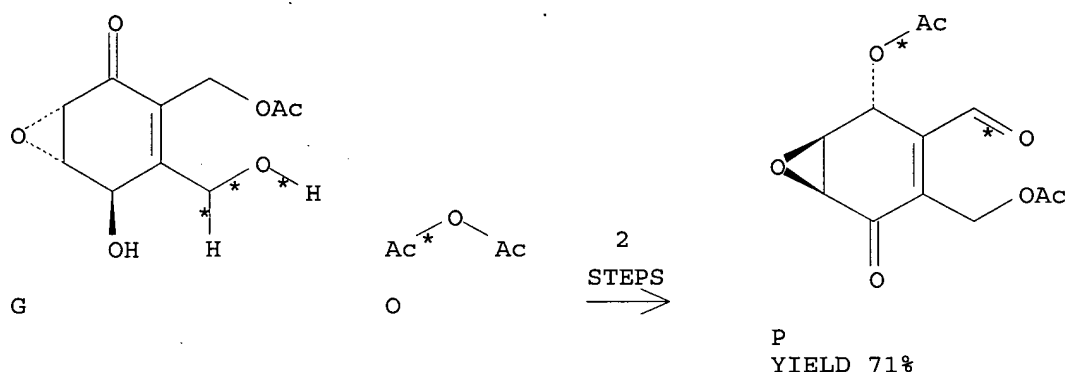
Updated Search

10509228

SOL 109-99-9 THF
CON -78 deg C
NTE regioselective, stereoselective

RX(3) RCT G 676263-76-6
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2
PRO J 676263-78-8
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

RX(14) OF 100 COMPOSED OF RX(3), RX(4)
RX(14) G + O ==> P



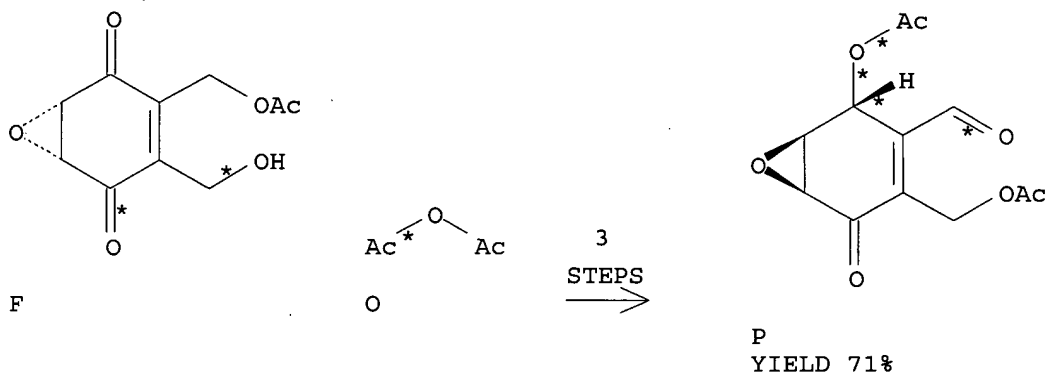
RX(3) RCT G 676263-76-6
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2
PRO J 676263-78-8
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

RX(4) RCT J 676263-78-8, O 108-24-7
RGT Q 110-86-1 Pyridine
PRO P 676263-80-2
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON 0 deg C
NTE stereoselective

RX(25) OF 100 COMPOSED OF RX(2), RX(3), RX(4)
RX(25) F + O ==> P

Updated Search

10509228



RX(2) RCT F 676263-74-4
 RGT H 1191-15-7 AlH(Bu-i)₂
 PRO G 676263-76-6
 SOL 109-99-9 THF
 CON -78 deg C
 NTE regioselective, stereoselective

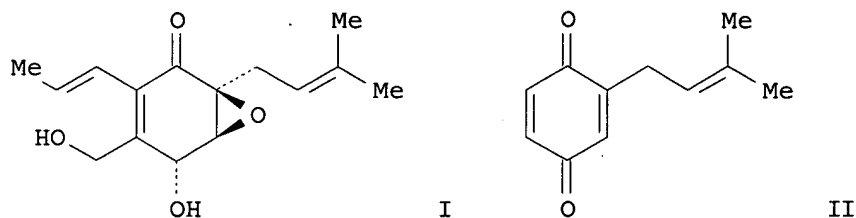
RX(3) RCT G 676263-76-6
 RGT K 2564-83-2 Me₄-piperidoxyl, L 7782-44-7 O₂
 PRO J 676263-78-8
 CAT 7758-89-6 CuCl
 SOL 68-12-2 DMF
 CON room temperature
 NTE chemoselective

RX(4) RCT J 676263-78-8, O 108-24-7
 RGT Q 110-86-1 Pyridine
 PRO P 676263-80-2
 CAT 1122-58-3 4-DMAP
 SOL 75-09-2 CH₂Cl₂
 CON 0 deg C
 NTE stereoselective

L3 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 140:270655 CASREACT
 TITLE: Total Synthesis of the Novel Antifungal Agent
 (±)-Jesterone
 AUTHOR(S): Mehta, Goverdhan; Pan, Subhas Chandra
 CORPORATE SOURCE: Department of Organic Chemistry, Indian Institute of
 Science, Bangalore, 560 012, India
 SOURCE: Organic Letters (2004), 6(5), 811-813
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

Updated Search

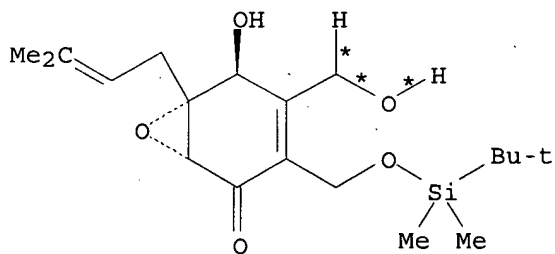
10509228



AB A total synthesis of the novel, biol. active epoxyquinone natural product (+)-jesterone (I) was accomplished via the formation of the Diels-Alder adduct of cyclopentadiene and prenylated 1,4-benzoquinone II. This approach is notable for its conceptual simplicity and efficient orchestration of a series of chemo-, regio-, and stereoselective operations.

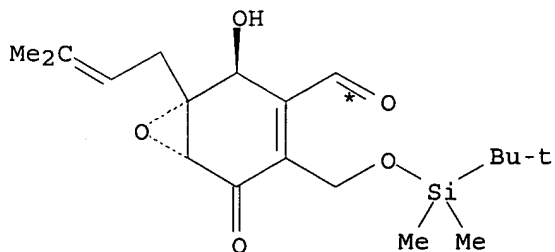
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 201 ...AF ==> AH...



AF

(11) →



AH
YIELD 90%

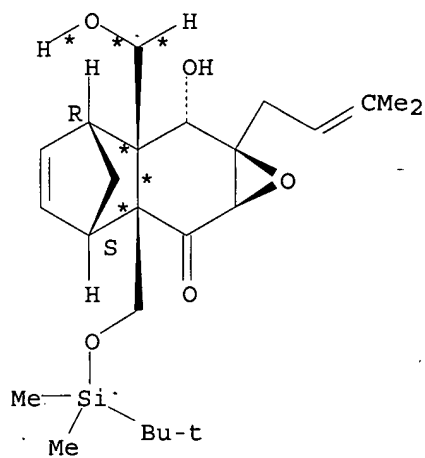
RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF

Updated Search

10509228

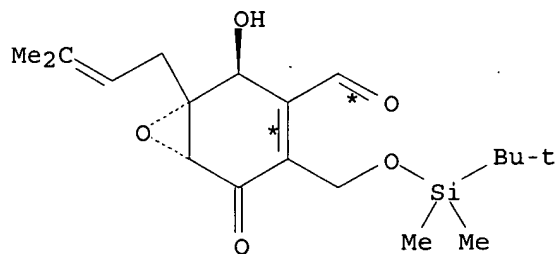
CON 3 hours, room temperature
NTE chemoselective

RX(26) OF 201 COMPOSED OF RX(10), RX(11)
RX(26) AD ==> AH



AD

2
STEPS
→



AH
YIELD 90%

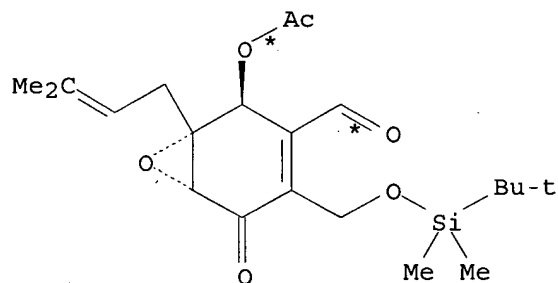
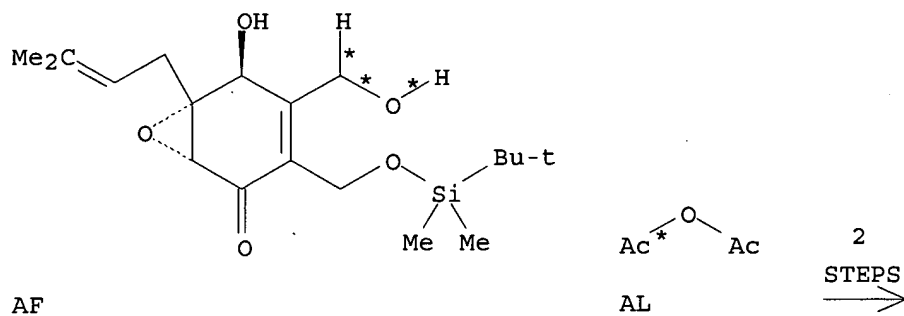
RX(10) RCT AD 674358-47-5
PRO AF 674358-50-0
SOL 101-84-8 PhOPh
CON 6 minutes, 220 deg C
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

Updated Search

10509228

RX(27) OF 201 COMPOSED OF RX(11), RX(12)
RX(27) AF + AL ==> AM



AM
YIELD 98%

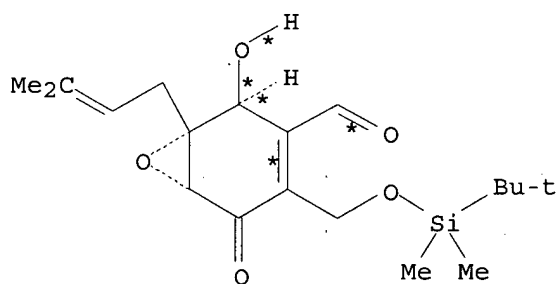
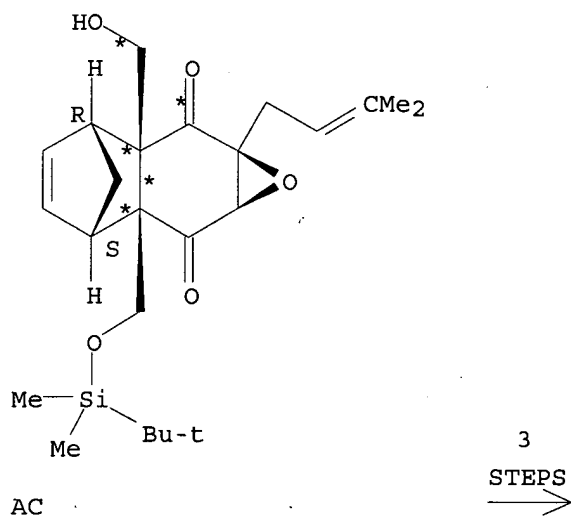
RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

RX(12) RCT AH 674358-53-3, AL 108-24-7
RGT AN 110-86-1 Pyridine
PRO AM 674358-56-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON 3 hours, 0 deg C

RX(48) OF 201 COMPOSED OF RX(9), RX(10), RX(11)
RX(48) AC ==> AH

Updated Search

10509228



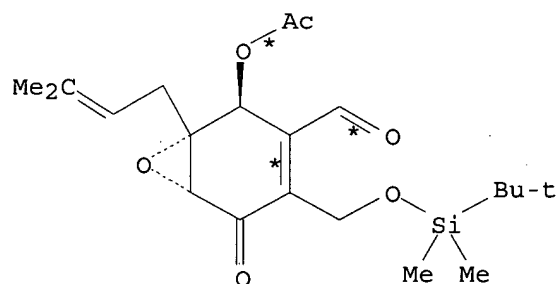
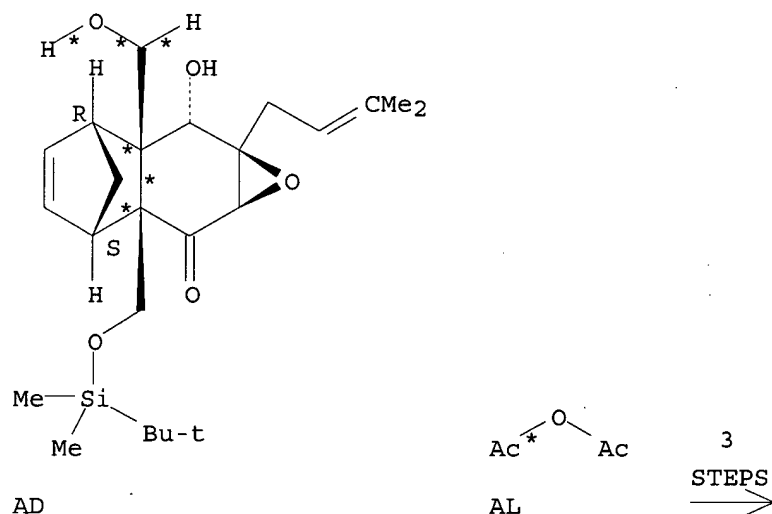
AH
YIELD 90%

RX(9)	RCT	AC 674358-44-2
	RGT	AE 16940-66-2 NaBH ₄
	PRO	AD 674358-47-5
	SOL	67-56-1 MeOH
	CON	1 hour, -5 deg C
	NTE	regioselective, stereoselective
RX(10)	RCT	AD 674358-47-5
	PRO	AF 674358-50-0
	SOL	101-84-8 PhOPh
	CON	6 minutes, 220 deg C
	NTE	chemoselective, retro-Diels-Alder reaction
RX(11)	RCT	AF 674358-50-0
	RGT	AI 2564-83-2 Me ₄ -piperidoxyl, AJ 7782-44-7 O ₂
	PRO	AH 674358-53-3
	CAT	7758-89-6 CuCl
	SOL	68-12-2 DMF
	CON	3 hours, room temperature
	NTE	chemoselective

Updated Search

10509228

RX(50) OF 201 COMPOSED OF RX(10), RX(11), RX(12)
 RX(50) AD + AL ==> AM



AM
 YIELD 98%

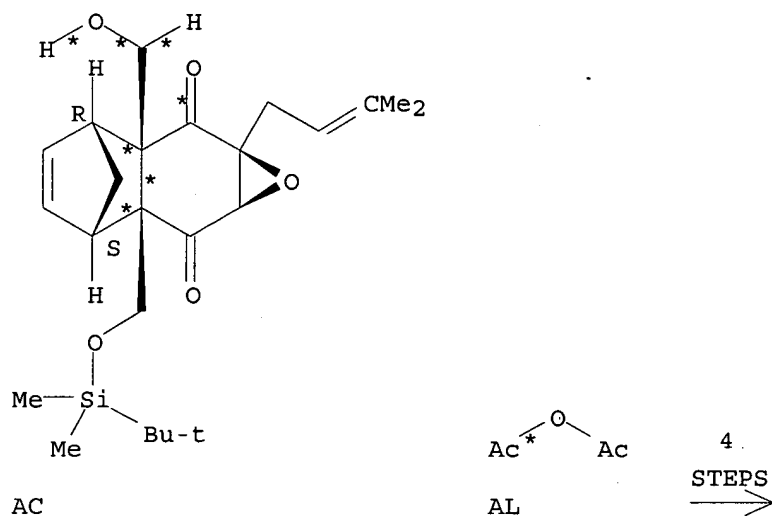
RX(10)	RCT	AD 674358-47-5
	PRO	AF 674358-50-0
	SOL	101-84-8 PhOPh
	CON	6 minutes, 220 deg C
	NTE	chemoselective, retro-Diels-Alder reaction
RX(11)	RCT	AF 674358-50-0
	RGT	AI 2564-83-2 Me ₄ -piperidoxyl, AJ 7782-44-7 O ₂
	PRO	AH 674358-53-3
	CAT	7758-89-6 CuCl
	SOL	68-12-2 DMF
	CON	3 hours, room temperature
	NTE	chemoselective
RX(12)	RCT	AH 674358-53-3, AL 108-24-7
	RGT	AN 110-86-1 Pyridine
	PRO	AM 674358-56-6

Updated Search

10509228

CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH₂Cl₂
CON 3 hours, 0 deg C

RX(51) OF 201 COMPOSED OF RX(9), RX(10), RX(11), RX(12)
RX(51) AC + AL ==> AM



AM
YIELD 98%

RX(9) RCT AC 674358-44-2
RGT AE 16940-66-2 NaBH₄
PRO AD 674358-47-5
SOL 67-56-1 MeOH
CON 1 hour, -5 deg C
NTE regioselective, stereoselective

RX(10) RCT AD 674358-47-5
PRO AF 674358-50-0
SOL 101-84-8 PhOPh
CON 6 minutes, 220 deg C
NTE chemoselective, retro-Diels-Alder reaction

Updated Search

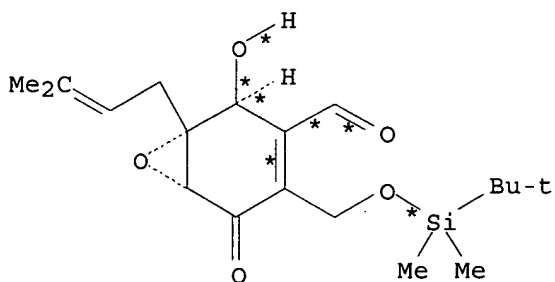
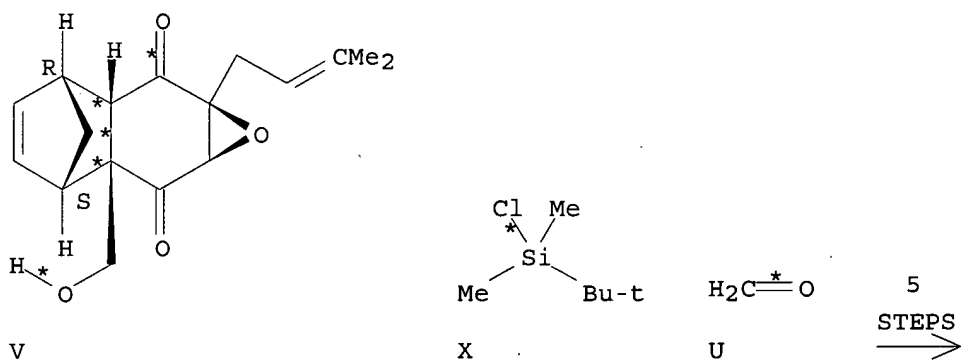
10509228

RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

RX(12) RCT AH 674358-53-3, AL 108-24-7
RGT AN 110-86-1 Pyridine
PRO AM 674358-56-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON 3 hours, 0 deg C

RX(83) OF 201 COMPOSED OF RX(7), RX(8), RX(9), RX(10), RX(11)

RX(83) V + X + U ==> AH



AH
YIELD 90%

RX(7) RCT V 674358-38-4, X 18162-48-6
RGT Z 1122-58-3 4-DMAP, AA 288-32-4 1H-Imidazole
PRO Y 674358-41-9
SOL 68-12-2 DMF
CON 0 deg C

RX(8) RCT Y 674358-41-9, U 50-00-0

Updated Search

10509228

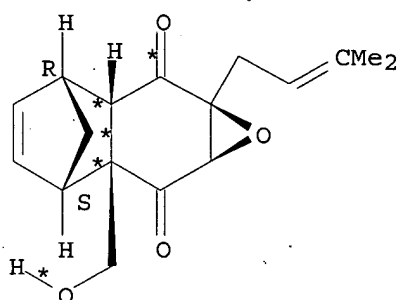
RGT W 6674-22-2 DBU
PRO AC 674358-44-2
SOL 7732-18-5 Water, 109-99-9 THF
CON 36 hours, 0 deg C

RX(9) RCT AC 674358-44-2
RGT AE 16940-66-2 NaBH4
PRO AD 674358-47-5
SOL 67-56-1 MeOH
CON 1 hour, -5 deg C
NTE regioselective, stereoselective

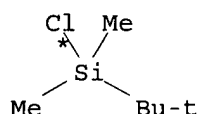
RX(10) RCT AD 674358-47-5
PRO AF 674358-50-0
SOL 101-84-8 PhOPh
CON 6 minutes, 220 deg C
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

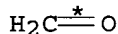
RX(88) OF 201 COMPOSED OF RX(7), RX(8), RX(9), RX(10), RX(11), RX(12)
RX(88) V + X + U + AL ==> AM



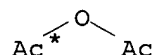
V



X



U



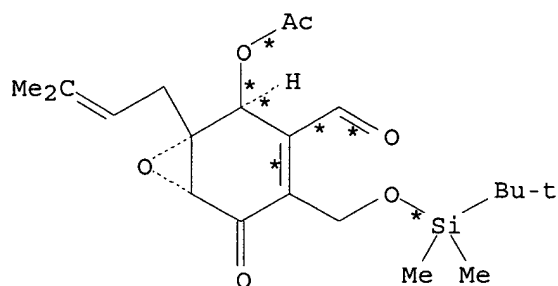
AL

6

STEPS
→

Updated Search

10509228



AM
YIELD 98%

RX(7) RCT V 674358-38-4, X 18162-48-6
RGT Z 1122-58-3 4-DMAP, AA 288-32-4 1H-Imidazole
PRO Y 674358-41-9
SOL 68-12-2 DMF
CON 0 deg C

RX(8) RCT Y 674358-41-9, U 50-00-0
RGT W 6674-22-2 DBU
PRO AC 674358-44-2
SOL 7732-18-5 Water, 109-99-9 THF
CON 36 hours, 0 deg C

RX(9) RCT AC 674358-44-2
RGT AE 16940-66-2 NaBH4
PRO AD 674358-47-5
SOL 67-56-1 MeOH
CON 1 hour, -5 deg C
NTE regioselective, stereoselective

RX(10) RCT AD 674358-47-5
PRO AF 674358-50-0
SOL 101-84-8 PhOPh
CON 6 minutes, 220 deg C
NTE chemoselective, retro-Diels-Alder reaction

RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

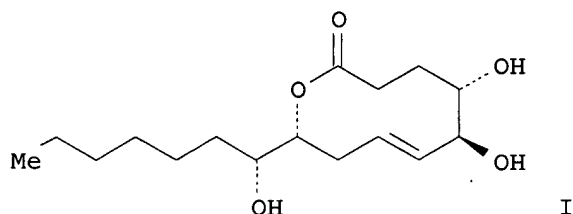
RX(12) RCT AH 674358-53-3, AL 108-24-7
RGT AN 110-86-1 Pyridine
PRO AM 674358-56-6
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON 3 hours, 0 deg C

L3 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:199131 CASREACT

Updated Search

10509228

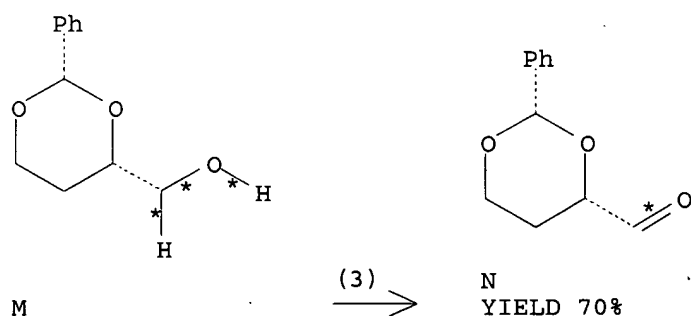
TITLE: Stereoselective total synthesis of the nonenolide
(+)-microcarpalide
AUTHOR(S): Banwell, Martin G.; Loong, David T. J.
CORPORATE SOURCE: Research School of Chemistry, Institute of Advanced
Studies, The Australian National University, Canberra,
ACT 0200, Australia
SOURCE: Heterocycles (2004), 62, 713-734
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The enantiomer, (+)-microcarpalide (I), of the nonenolide natural product
(+)-microcarpalide has been prepared from (S)-malic acid and 3-decyn-1-ol
via a sixteen step sequence involving ring closing metathesis (RCM).

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 288 ...M ==> N...



RX(3) RCT M 103773-79-1

STAGE(1)

RGT O 3240-34-4 PhI(OAc)₂, P 14691-89-5
1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-
SOL 75-09-2 CH₂Cl₂
CON 14 hours, 18 deg C

STAGE(2)

RGT E 144-55-8 NaHCO₃

Updated Search

10509228

SOL 7732-18-5 Water
CON 18 deg C

PRO N 145958-02-7

L3 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:111158 CASREACT

TITLE: Milbemycin α 17 and related compounds synthesized from milbemycin A4: Synthetic procedure and acaricidal activities

AUTHOR(S): Tsukiyama, Takahiro; Kinoshita, Ayakoe; Ichinose, Reiji; Sato, Kazuo

CORPORATE SOURCE: Agrosience Research Laboratories, Sankyo Agro Co., Ltd., Shiga, 520-2342, Japan

SOURCE: Journal of Antibiotics (2003), 56(10), 848-855
CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

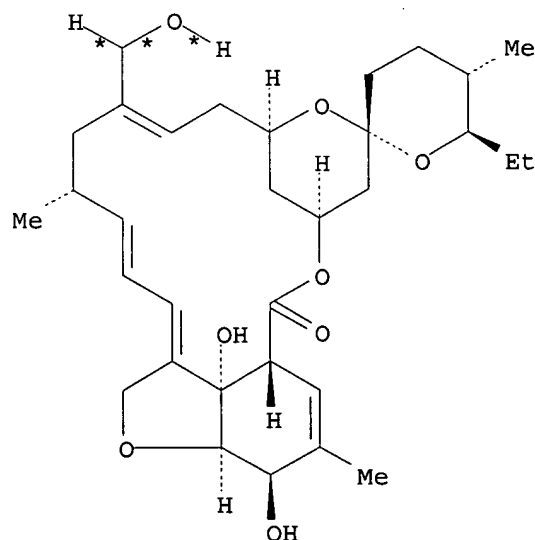
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Milbemycin α 17 (I), a 14-demethyl congener of milbemycin A4, has been reported as a natural product. In this paper, we report the successful development of a chemical derivation method to synthesize milbemycin α 17 from milbemycin A4, as well as our use of a similar method to prepare 24-demethylmilbemycin A4' from the same precursor. Thus, I was prepared by desilylation of the 5-O-TBDMS ether which was prepared by decarbonylation of 5-O-TBDMS-14-formylmilbemycin A4. The acaricidal activities of these compds. were assessed against the organophosphorus-sensitive two-spotted spider mites (*Tetranychus urticae*) on the primary leaves of cowpea plants (*Vigna sinensis* Savi species) by spraying.

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 28 ...K ==> M...

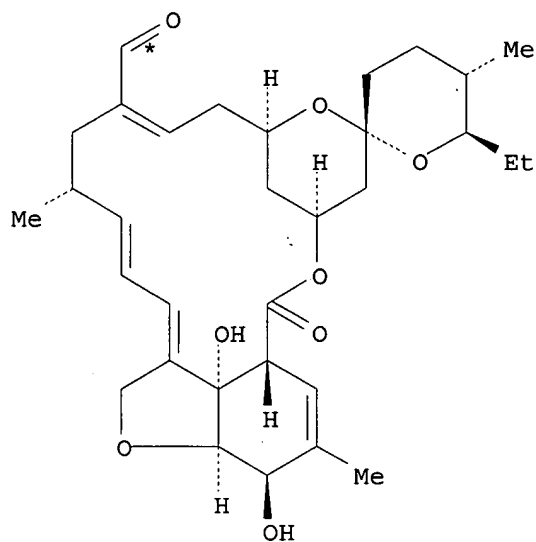


K

(5) \rightarrow

Updated Search

10509228



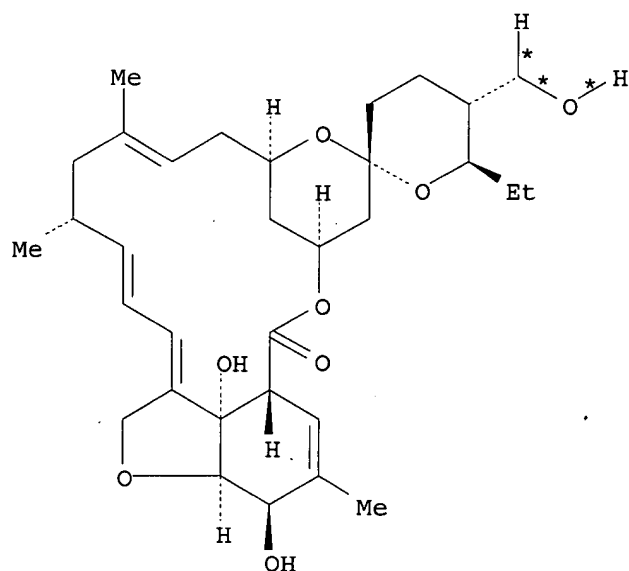
M
YIELD 87%

RX(5) RCT K 112774-81-9
RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NCl, R 128-09-6
Chlorosuccinimide
PRO M 112774-92-2
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 1 hour, room temperature
NTE regioselective

RX(9) OF 28 AB ==> AC...

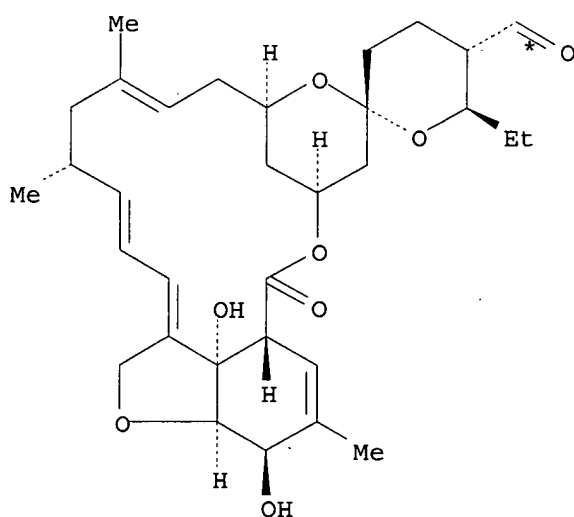
Updated Search

10509228



AB

(9) →



AC

YIELD 53%

RX(9)

RCT AB 123022-52-6

RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NCl, R 128-09-6
Chlorosuccinimide

PRO AC 482621-67-0

SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂

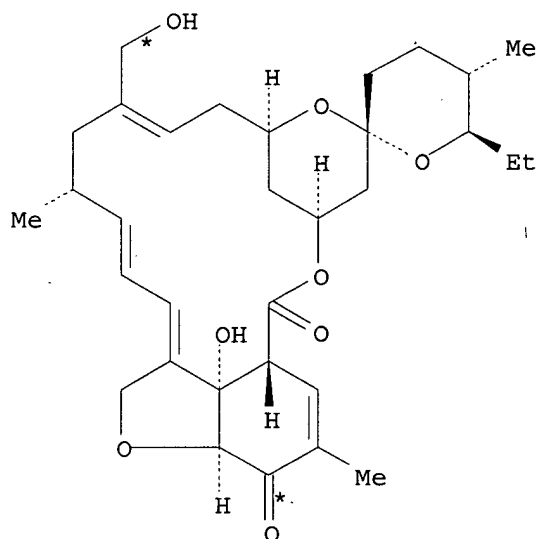
CON 1 hour, room temperature

NTE regioselective

Updated Search

10509228

RX(13) OF 28 COMPOSED OF RX(4), RX(5)
RX(13) G ==> M



2
STEPS
→

G

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

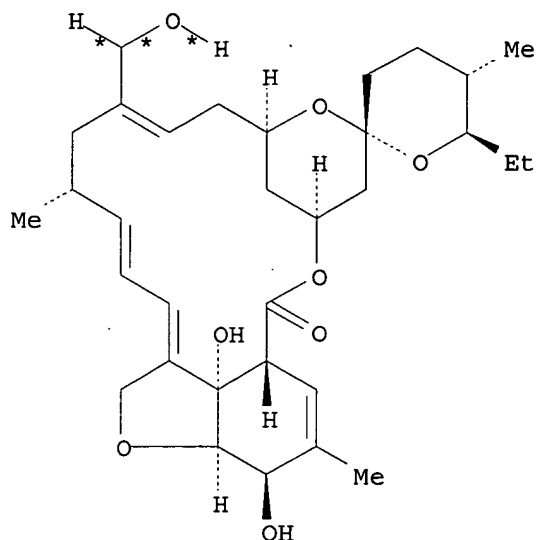
RX(4) RCT G 141547-92-4
RGT L 16940-66-2 NaBH4
PRO K 112774-81-9
SOL 67-56-1 MeOH
CON 10 minutes, 0 deg C
NTE stereoselective

RX(5) RCT K 112774-81-9
RGT N 144-55-8 NaHCO3, O 584-08-7 K2CO3, P 2564-83-2
Me4-piperidoxyl, Q 1112-67-0 Bu4NCl, R 128-09-6
Chlorosuccinimide
PRO M 112774-92-2
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 1 hour, room temperature
NTE regioselective

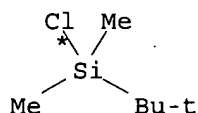
RX(14) OF 28 COMPOSED OF RX(5), RX(6)
RX(14) K + T ==> U

Updated Search

10509228



K



T

2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

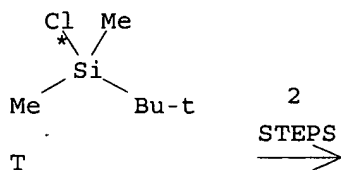
RX(5) RCT K 112774-81-9
RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NCl, R 128-09-6
Chlorosuccinimide
PRO M 112774-92-2
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 1 hour, room temperature
NTE regioselective

RX(6) RCT M 112774-92-2, T 18162-48-6
RGT V 288-32-4 1H-Imidazole
PRO U 112774-91-1
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(17) OF 28 COMPOSED OF RX(9), RX(10)

RX(17) AB + T ==> AD

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



T

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

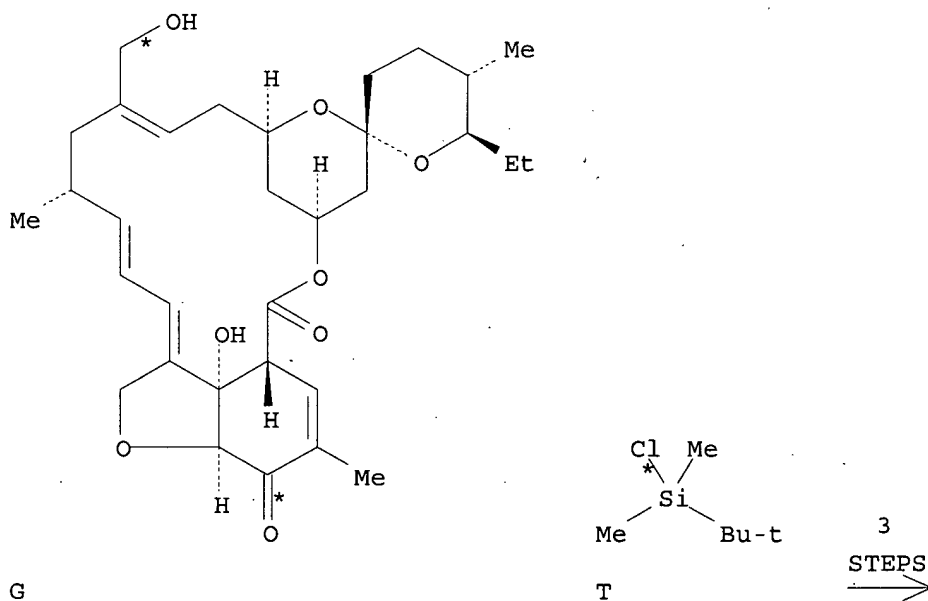
Updated Search

10509228

RX(9) RCT AB 123022-52-6
RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NC₁, R 128-09-6
Chlorosuccinimide
PRO AC 482621-67-0
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 1 hour, room temperature
NTE regioselective

RX(10) RCT AC 482621-67-0, T 18162-48-6
RGT V 288-32-4 1H-Imidazole
PRO AD 482621-71-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

RX(20) OF 28 COMPOSED OF RX(4), RX(5), RX(6)
RX(20) G + T ==> U



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT G 141547-92-4
RGT L 16940-66-2 NaBH₄
PRO K 112774-81-9
SOL 67-56-1 MeOH
CON 10 minutes, 0 deg C
NTE stereoselective

RX(5) RCT K 112774-81-9
RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NC₁, R 128-09-6
Chlorosuccinimide
PRO M 112774-92-2

Updated Search

10509228

SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 1 hour, room temperature
NTE regioselective

RX(6) RCT M 112774-92-2, T 18162-48-6
RGT V 288-32-4 1H-Imidazole
PRO U 112774-91-1
SOL 68-12-2 DMF
CON 3 hours, room temperature

L3 ANSWER 23 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:337963 CASREACT

TITLE: Oxidation and reduction process for the preparation of
5-formyl-4-methylthiazole

INVENTOR(S): Deshpande, Pandurang Balwant; Luthra, Parven Kumar;
Vyas, Rajesh; Kamma, Ramakrishna

PATENT ASSIGNEE(S): Orchid Chemicals & Pharmaceuticals Limited, India

SOURCE: U.S. Pat. Appl. Publ., 4 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

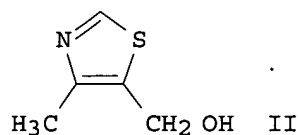
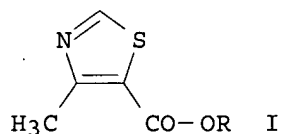
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003204095	A1	20031030	US 2002-309812	20021205
US 6833459	B2	20041221		
IN 194928	A	20041211	IN 2002-MA325	20020426
CA 2483482	AA	20031106	CA 2002-2483482	20021210
WO 2003091230	A1	20031106	WO 2002-IB5270	20021210
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002367890	A1	20031110	AU 2002-367890	20021210
CN 1628108	A	20050615	CN 2002-829187	20021210
JP 2005526112	T2	20050902	JP 2003-587790	20021210
PRIORITY APPLN. INFO.:			IN 2002-MA325	20020426
			WO 2002-IB5270	20021210

OTHER SOURCE(S): MARPAT 139:337963

GI

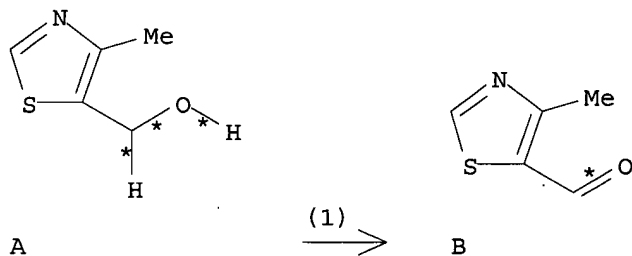
10509228



AB 4-Methyl-5-formylthiazole is prepd in high yield and selectivity by the reduction of the corresponding ester (I; R = C1-4 alkyl; e.g., Et 4-methyl-5-thiazolecarboxylate) into 5-(hydroxymethyl)-4-methylthiazole (II) which is then subjected to liquid-phase oxidation to give the product aldehyde.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 5 ...A ==> B



RX(1) RCT A 1977-06-6

STAGE(1)

SOL 75-09-2 CH₂Cl₂

CON 5 minutes, room temperature

STAGE(2)

RGT C 144-55-8 NaHCO₃

SOL 7732-18-5 Water

CON SUBSTAGE(1) 30 - 32 deg C

SUBSTAGE(2) 5 - 10 minutes, 30 - 32 deg C

STAGE(3)

RGT D 7758-02-3 KBr, E 2564-83-2 Me₄-piperidoxyl, F

7681-52-9 NaOCl

SOL 7732-18-5 Water

CON SUBSTAGE(1) 32 deg C -> 0 deg C

Updated Search

10509228

SUBSTAGE(3) 1 hour, 0 - 2 deg C
SUBSTAGE(4) 0 - 2 deg C

PRO B 82294-70-0

L3 ANSWER 24 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 138:24587 CASREACT

TITLE: Process for the preparation of prostaglandins and analogs

INVENTOR(S): Greenwood, Alan Kenneth; McHattie, Derek; Thompson, David George; Clissold, Derek Wyndham

PATENT ASSIGNEE(S): Resolution Chemicals Limited, UK; Cascade Biochem Limited

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

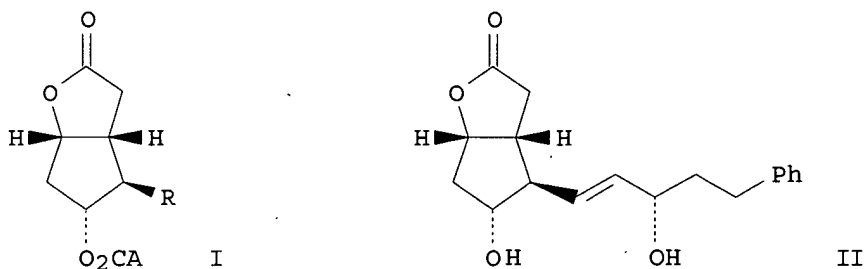
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096898	A2	20021205	WO 2002-GB2462	20020524
WO 2002096898	A3	20030320		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2448088	AA	20021205	CA 2002-2448088	20020524
NZ 529634	A	20031219	NZ 2002-529634	20020524
EP 1389198	A2	20040218	EP 2002-755096	20020524
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2002009984	A	20040406	BR 2002-9984	20020524
CN 1533385	A	20040929	CN 2002-814634	20020524
JP 2005503354	T2	20050203	JP 2003-500077	20020524
US 2004249172	A1	20041209	US 2004-478513	20040608
US 2005261374	A1	20051124	US 2005-189985	20050727
US 2005272877	A1	20051208	US 2005-189986	20050727
PRIORITY APPLN. INFO.:			GB 2001-12699	20010524
			WO 2002-GB2462	20020524
			US 2004-478513	20040608

OTHER SOURCE(S): MARPAT 138:24587

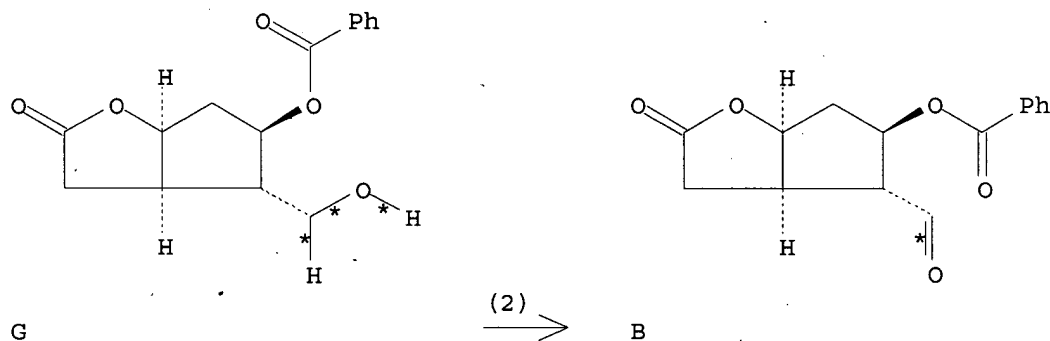
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AB The formylloxabicyclooctanones I (A = C6-10-aryl which may be substituted by halo, alkyl, aryl) were prepared by oxidation of the corresponding alcs. as intermediates for prostaglandin synthesis especially analogs of PGF₂α. Thus, (-)-benzyl Corey lactone (I, R = CH₂OH, A = Ph) was treated with NaOCl, TEMPO and KBr in CH₂Cl₂ to give I (R = CHO, A = Ph), which was converted to latanoprost in several steps by standard methods, via derivative II.

RX(2) OF 66 G ==> B...



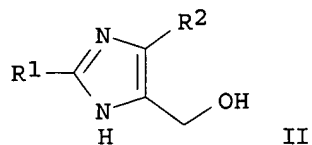
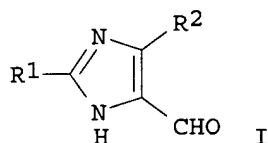
RX(2) RCT G 39746-00-4
 RGT H 7681-52-9 NaOCl, I 2564-83-2 Me₄-piperidoxyl, J 7758-02-3 KBr
 PRO B 39746-01-5
 SOL 75-09-2 CH₂Cl₂

L3 ANSWER 25 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 137:247693 CASREACT
 TITLE: Preparation of 4-formylimidazoles
 INVENTOR(S): Isokawa, Sorou; Enomoto, Katashi; Nagai, Naoshi
 PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

Updated Search

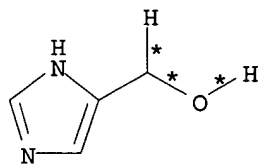
10509228

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275162	A2	20020925	JP 2001-73700	20010315
PRIORITY APPLN. INFO.:			JP 2001-73700	20010315
OTHER SOURCE(S):			MARPAT 137:247693	
GI				



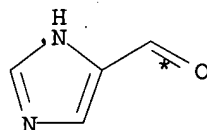
AB The compds. I [R1, R2 = H, C1-10 (un)substituted alkyl, aryl, halo] are prepared by reaction of imidazoles II (R1, R2 = same as I) in the presence of 2,2,6,6-tetramethylpiperidine N-oxyls and cooxidizing agents in organic solvents or water solvents under basic condition.

RX(1) OF 3 A ==> B



● HCl

A



B
YIELD 57%

RX(1) RCT A 32673-41-9

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,
4-hydroxy-2,2,6,6-tetramethyl-
SOL 75-09-2 CH2Cl2

STAGE(2)

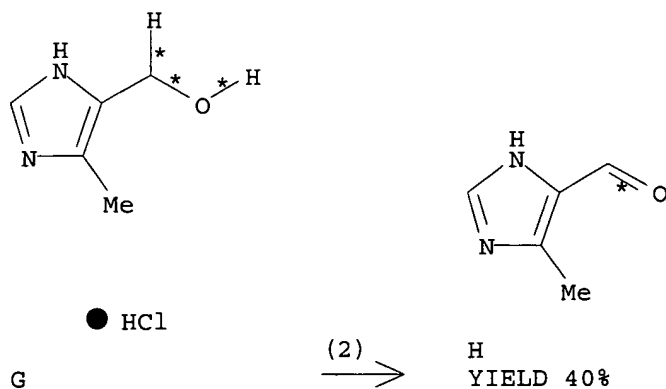
RGT D 7681-52-9 NaOCl
SOL 7732-18-5 Water

PRO B 3034-50-2

RX(2) OF 3 G ==> H

Updated Search

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RX(2) RCT G 38585-62-5

STAGE(1)

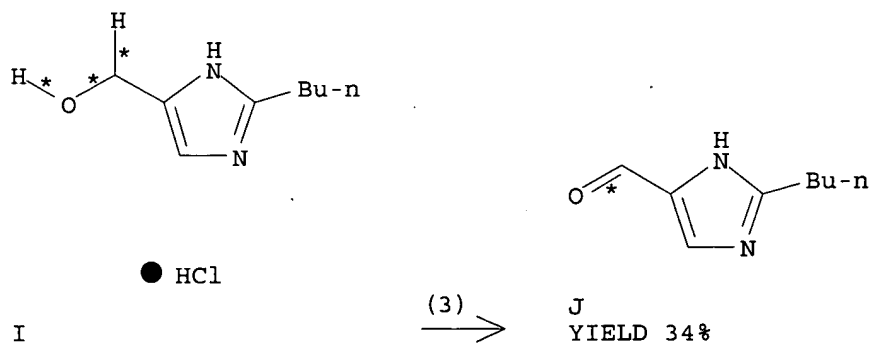
RGT C 2226-96-2 1-Piperidinyloxy,
4-hydroxy-2,2,6,6-tetramethyl-
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT D 7681-52-9 NaOCl
SOL 7732-18-5 Water

PRO H 68282-53-1

RX(3) OF 3 I ==> J



RX(3) RCT I 460717-19-5

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,
4-hydroxy-2,2,6,6-tetramethyl-
CAT 71-91-0 Et₄N.Br
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT D 7681-52-9 NaOCl
SOL 7732-18-5 Water

Updated Search

10509228

PRO J 68282-49-5

L3 ANSWER 26 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 137:201293 CASREACT
TITLE: Method of synthesizing camptothecin-relating compounds
INVENTOR(S): Ogawa, Takanori; Nishiyama, Hiroyuki; Uchida, Miyuki;
Sawada, Seigo
PATENT ASSIGNEE(S): Kabushiki Kaisha Yakult Honsha, Japan
SOURCE: PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002066416	A1	20020829	WO 2002-JP1538	20020221
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2437702	AA	20020829	CA 2002-2437702	20020221
EE 200300373	A	20031015	EE 2003-373	20020221
EP 1378505	A1	20040107	EP 2002-703874	20020221
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
CN 1492851	A	20040428	CN 2002-805323	20020221
NZ 527615	A	20041224	NZ 2002-527615	20020221
BG 108031	A	20050430	BG 2003-108031	20030725
ZA 2003006223	A	20040603	ZA 2003-6223	20030812
NO 2003003579	A	20031010	NO 2003-3579	20030813
NZ 534374	A	20041224	NZ 2003-534374	20030814
US 2004106830	A1	20040603	US 2003-467987	20031218
PRIORITY APPLN. INFO.:			JP 2001-45430	20010221
			JP 2001-309322	20011005
			JP 2001-309332	20011005
			WO 2002-JP1538	20020221
OTHER SOURCE(S):	MARPAT 137:201293			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

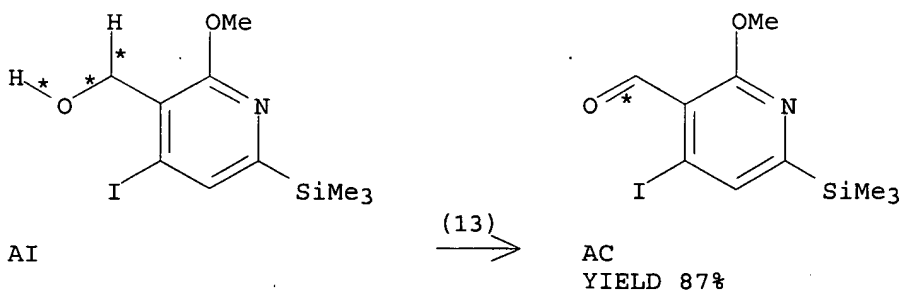
AB 2'-Amino-5'-hydroxypropiophenone (I) corresponding to the AB cycle moiety of the camptothecin (CPT) skeleton and a tricyclic ketone, namely (S)-4-ethyl-7,8-dihydro-4-hydroxy-1H-pyrano[3,4-f]indolizine-3,6,10(4H)-trione (II) corresponding to the CDE cycle moiety thereof can be efficiently produced and thus CPT and its derivs. can be stably supplied by a practically usable total synthesis to more efficiently provide

Updated Search

camptothecin (CPT), which is a starting compound for irinotecan hydrochloride, namely 7-ethyl-10-[4-(1-piperidino)-1-piperidino]carbonyloxycamptothecin hydrochloride trihydrate, and various camptothecin derivs. Thus, benzylation of 2-nitro-5-hydroxybenzaldehyde by benzyl chloride in the presence of K₂CO₃ in DMF at 60° for 20 h gave 94% 5-benzyloxy-2-nitrobenzaldehyde which went addition reaction with vinylmagnesium bromide in THF at 3-10° for 1 h to give 84.0% 1-(5-benzyloxy-2-nitrophenyl)-2-propen-1-ol (VIII). Oxidation of VIII with MnO₂ in CHCl₃ at 25° for 15 h gave 91% 1-(5-benzyloxy-2-nitrophenyl)-1-oxo-2-propene which was hydrogenated over 10% Pd-C in EtOAc under H atmospheric for 13 h to give 81% I. K₂OsO₄·2H₂O and (DHQD)2Pyr were added to an aqueous solution of K₃Fe(CN)₆, K₂CO₃, and MeSO₂NH₂ and stirred at .apprx.5° for 1 h, followed by adding 4-ethyl-8-methoxy-6-(trimethylsilyl)-1H-pyrano[3,4-c]pyridine, and the resulting mixture was stirred at 5° for 20 h, treated with sodium sulfite, and stirred at 5° for 30 min for asym. dihydroxylation to give a diol (III) (95%) which was oxidized by iodine and K₂CO₃ in aqueous methanol at 40° for 48 h to give a lactone (IV; R = TMS) (88%). Iodination of IV (R = TMS) by iodine and CF₃CO₂Ag in CH₂Cl₂ at room temperature for 16.5 h gave IV (R = iodo) (97%) which underwent carbonylation by CO in the presence of Pd(OAc)₂ and K₂CO₃ in 1-propanol at 60° for 18 to give an ester IV (R = n-PrO₂C) (70%). Demethylation of IV (R = n-PrO₂C) by treatment with Me₃SiCl and NaI in MeCN at room temperature for 3 h gave a keto lactone, namely 4-ethyl-3,4,7,8-tetrahydro-4-hydroxy-3,8-dioxo-1H-pyrano[3,4-c]pyridine-6-carboxylic acid Pr ester (V) (95%) which was cyclocondensed with tert-Bu acrylate in the presence of K₂CO₃ in DMSO at 50° for 20 min to give a tricyclic compound (VI) (77%). VI was heated with a mixture of CF₃CO₂H and PhMe at 110° for 100 min to give 77% II which was cyclocondensed with I in a 1:1 mixture of AcOH and toluene in the presence of p-toluenesulfonic acid monohydrate at 100° for 18 h to give SN-38 (VII; R₁ = H). VII (R₁ = H) was converted into irinotecan hydrochloride, VII.HCl (R₁ = Q).

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(13) OF 249 AI ==> AC



RX(13) RCT AI 375346-05-7
RGT AO 7681-52-9 NaOCl, AP 2564-83-2 Me4-piperidoxyl
PRO AC 174092-75-2
SOL 7732-18-5 Water, 108-88-3 PhMe
NTE oxidn. at 0-5° for 2 h

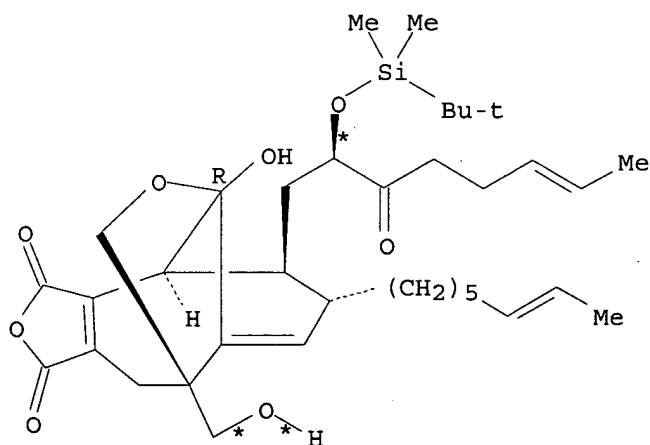
L3 ANSWER 27 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

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10509228

ACCESSION NUMBER: 136:325339 CASREACT
TITLE: Total Synthesis of the CP-Molecules (CP-263,114 and CP-225,917, Phomoidrides B and A). 2. Model Studies for the Construction of Key Structural Elements and First-Generation Strategy
AUTHOR(S): Nicolaou, K. C.; Baran, P. S.; Zhong, Y.-L.; Fong, K. C.; Choi, H.-S.
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (2002), 124(10), 2190-2201
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Crucial model synthetic and mechanistic studies directed toward the development of methodol. for the construction of the maleic anhydride moiety of the title CP-mols. are described. Studies directed toward the stereoselective attachment of the upper side chain, culminating in the discovery of long-range stereochem. control, are also discussed. In addition, a first-generation strategy toward the CP-mols., establishing a tricyclic diketone key intermediate as a "beachhead" from which all future operations would diverge, is also presented. Although this first-generation strategy failed to yield the target mols., the endeavor laid the important groundwork for the next-generation drives toward the CP-mols.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

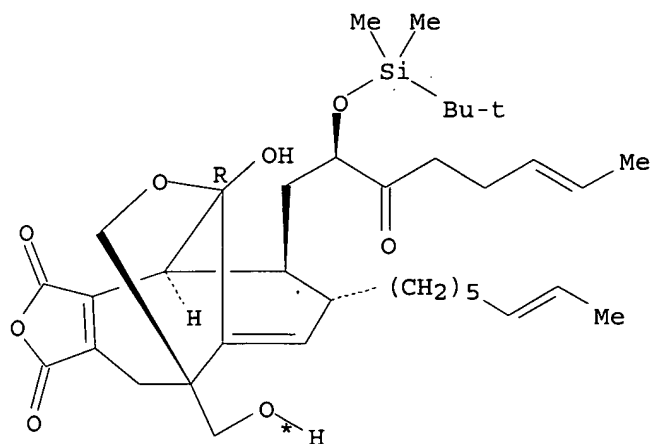
RX(362) OF 443 COMPOSED OF RX(38), RX(39), RX(40), RX(1), RX(43)
RX(362) 2 I + 2 BX + BA ==> DI



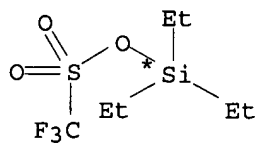
I

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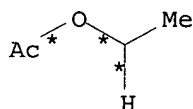
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I

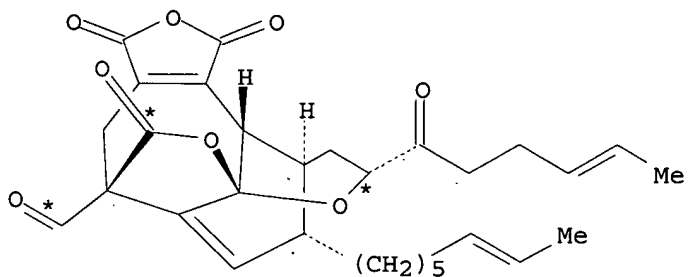


2 BX



BA

5
STEPS
→



DI

YIELD 95%

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

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STAGE(1)

RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4
PhI(OAc)2
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3
SOL 75-09-2 CH2Cl2

STAGE(2)

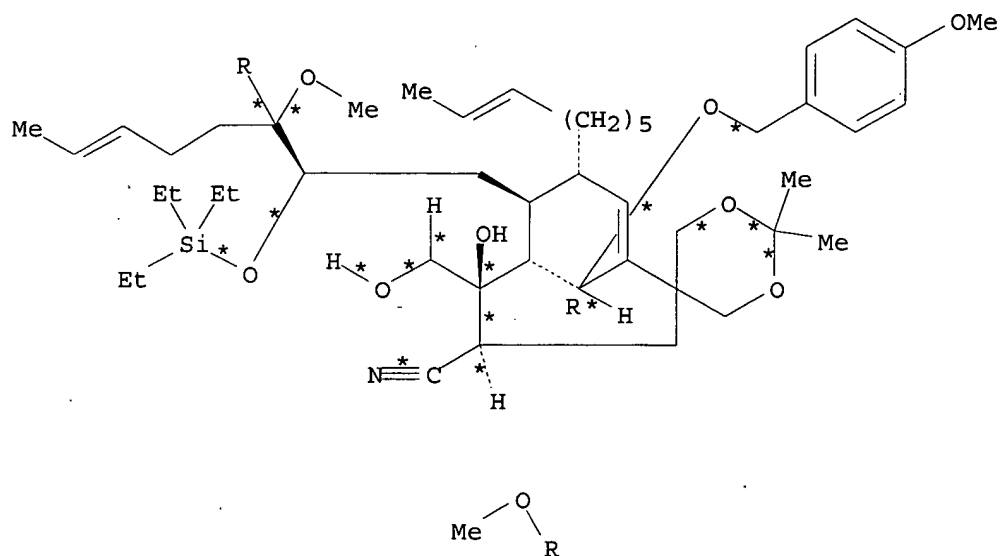
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

RX(367) OF 443 COMPOSED OF RX(28), RX(3), RX(36), RX(37), RX(2), RX(38),
RX(39), RX(40), RX(1), RX(43)

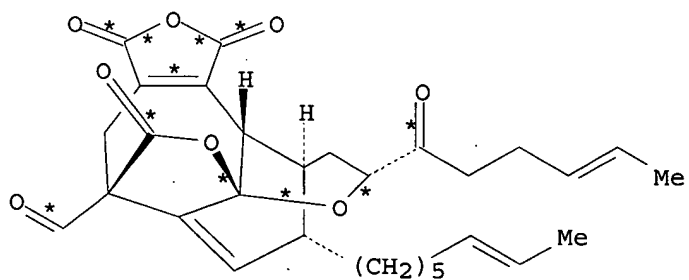
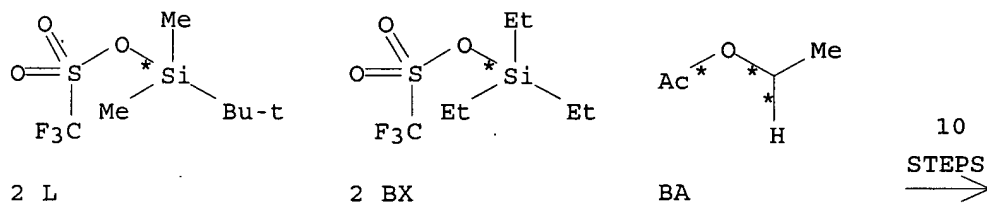
RX(367) 2 CJ + 2 L + 2 BX + BA ==> DI

10509228



CJ

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DI
YIELD 95%

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO2Cl, AC 121-44-8 Et3N

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10509228

SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K₂CO₃

SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O₂

SOL 60-29-7 Et₂O

STAGE(4)

RGT AF 144-62-7 (CO₂H)₂

PRO K 241819-21-6

NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me₂C(OMe)₂

CAT 3144-16-9 10-CSA

SOL 75-09-2 CH₂Cl₂

STAGE(3)

RCT L 69739-34-0

RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ

SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9

RGT BG 20039-37-6 PDC

PRO H 241819-25-0

SOL 75-09-2 CH₂Cl₂

RX(2) RCT H 241819-25-0

PRO I 241819-26-1

SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

Updated Search

10509228

STAGE(1)
RGT O 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)
RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)
RCT BA 141-78-6
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)
RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4
PhI(OAc)2
SOL 75-05-8 MeCN

STAGE(2)
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)
RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)
RGT D 75-75-2 MeSO3H
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)
RGT P 144-55-8 NaHCO3
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

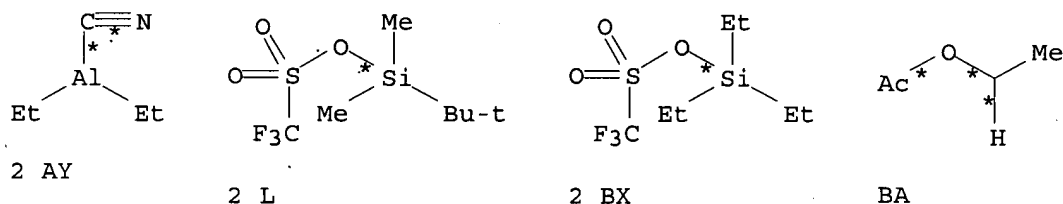
Updated Search

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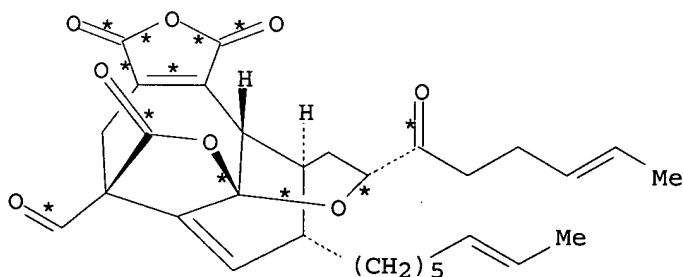
RX(368) OF 443 COMPOSED OF RX(27), RX(28), RX(3), RX(36), RX(37), RX(2),
RX(38), RX(39), RX(40), RX(1), RX(43)
RX(368) 2 CI + 2 AY + 2 L + 2 BX + BA ==> DI

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11
STEPS
→



DI
YIELD 95%

RX(27) RCT CI 241819-46-5, AY 5804-85-3
PRO CJ 412943-08-9
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO₂Cl, AC 121-44-8 Et₃N
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K₂CO₃
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O₂
SOL 60-29-7 Et₂O

STAGE(4)

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10509228

RGT AF 144-62-7 (CO₂H)₂

PRO K 241819-21-6

NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me₂C(OMe)₂

CAT 3144-16-9 10-CSA

SOL 75-09-2 CH₂Cl₂

STAGE(3)

RCT L 69739-34-0

RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ

SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9

RGT BG 20039-37-6 PDC

PRO H 241819-25-0

SOL 75-09-2 CH₂Cl₂

RX(2) RCT H 241819-25-0

PRO I 241819-26-1

SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

Updated Search

10509228

STAGE(1)

RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4
PhI(OAc)2
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3
SOL 75-09-2 CH2Cl2

STAGE(2)

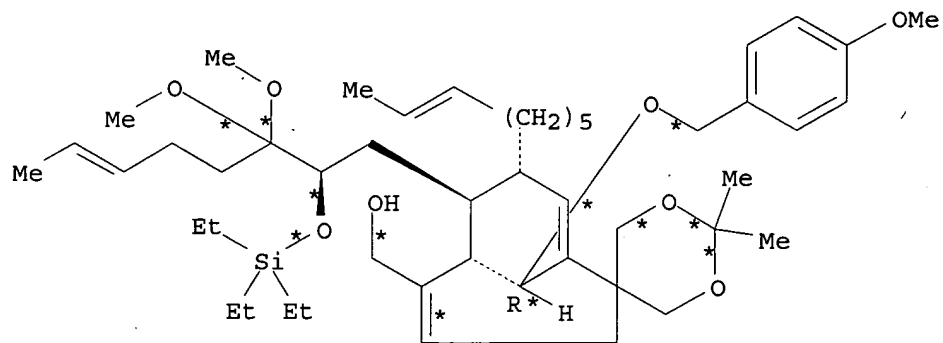
RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

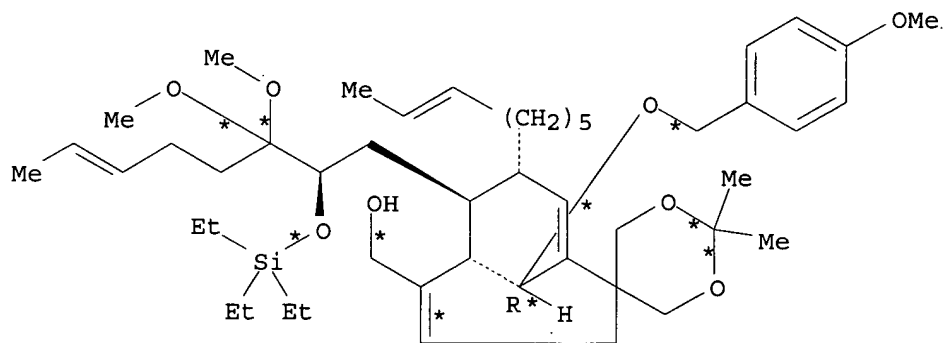
RX(369) OF 443 COMPOSED OF RX(26), RX(27), RX(28), RX(3), RX(36), RX(37),
RX(2), RX(38), RX(39), RX(40), RX(1), RX(43)

RX(369) 2 CH + 2 AY + 2 L + 2 BX + BA ==> DI

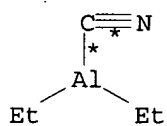
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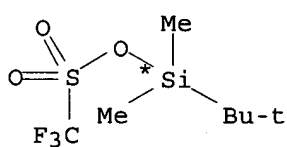
CH



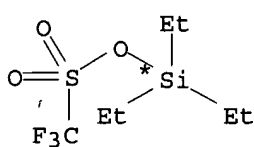
CH



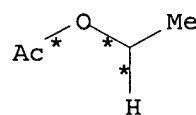
2 AY



2 L

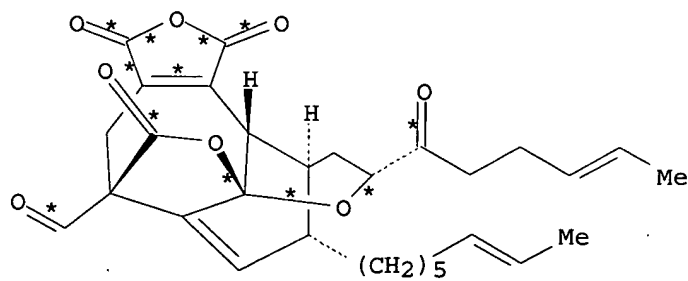


2 BX



BA

12
STEPS
→



DI
YIELD 95%

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10509228

RX(26) RCT CH 241819-19-2
RGT AT 75-91-2 t-BuOOH
PRO CI 241819-46-5
CAT 3153-26-2 VO acetylacetonate
SOL 71-43-2 Benzene, 124-18-5 Decane

RX(27) RCT CI 241819-46-5, AY 5804-85-3
PRO CJ 412943-08-9
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO₂Cl, AC 121-44-8 Et₃N
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K₂CO₃
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O₂
SOL 60-29-7 Et₂O

STAGE(4)

RGT AF 144-62-7 (CO₂H)₂

PRO K 241819-21-6
NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me₂C(OMe)₂
CAT 3144-16-9 10-CSA
SOL 75-09-2 CH₂Cl₂

STAGE(3)

RCT L 69739-34-0
RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO₃

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SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9
RGT BG 20039-37-6 PDC
PRO H 241819-25-0
SOL 75-09-2 CH₂Cl₂

RX(2) RCT H 241819-25-0
PRO I 241819-26-1
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6
RGT P 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me₄-piperidoxyl, DE 3240-34-4
PhI(OAc)₂
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F₃CCO₂H
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO₃H
SOL 67-66-3 CHCl₃

Updated Search

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PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3

SOL 75-09-2 CH2Cl2

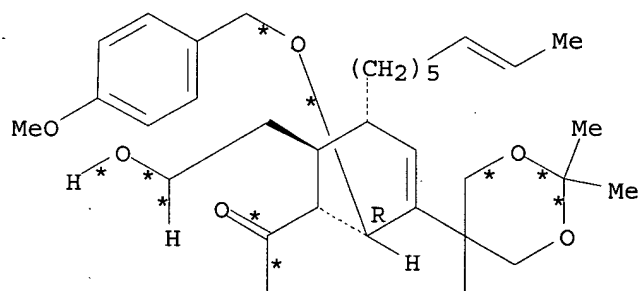
STAGE(2)

RGT BS 87413-09-0 Martin's reagent

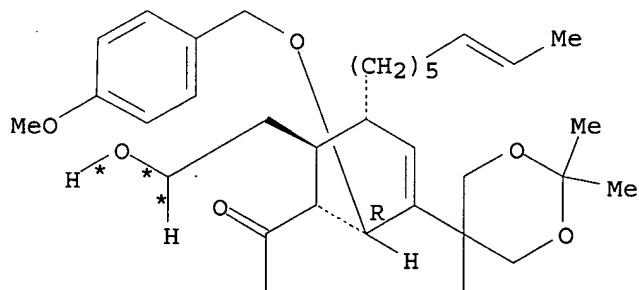
PRO DI 241819-31-8

RX(442) OF 443 COMPOSED OF RX(19), RX(20), RX(21), RX(22), RX(23), RX(24),
RX(25), RX(26), RX(27), RX(28), RX(3), RX(36), RX(37), RX(2), RX(38),
RX(39), RX(40), RX(1), RX(43)

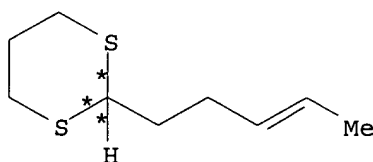
RX(442) 2 BP + 2 BT + 5 BX + S + 3 AI + 2 AG + 2 AY +
2 L + BA ==> DI



BP



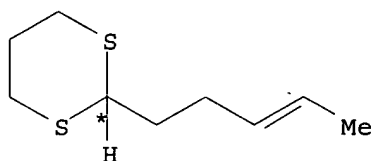
BP



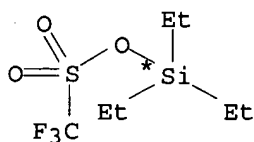
BT

Updated Search

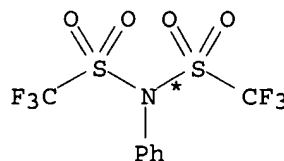
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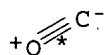
BT



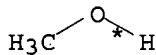
5 BX



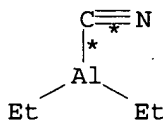
S



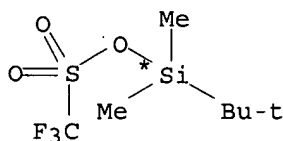
3 AI



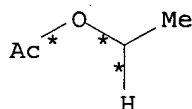
2 AG



2 AY

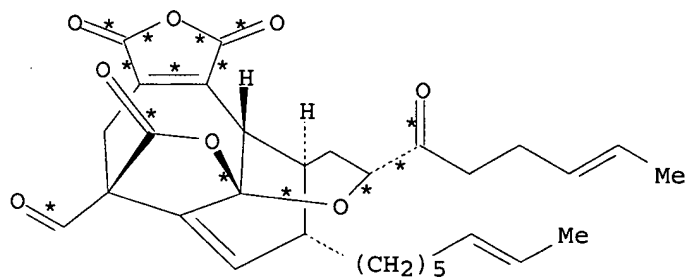


2 L



BA

19
STEPS
→



DI

YIELD 95%

RX(19) RCT BP 412943-02-3
RGT P 144-55-8 NaHCO₃, BS 87413-09-0 Martin's reagent
PRO BR 241819-12-5
SOL 75-09-2 CH₂Cl₂

RX(20) RCT BT 241819-10-3

STAGE(1)

RGT BV 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane

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STAGE(2)

RCT BR 241819-12-5
SOL 109-99-9 THF

STAGE(3)

RGT AM 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO BU 412943-03-4
NTE stereoselective

RX(21) RCT BU 412943-03-4

STAGE(1)

RGT CA 7646-69-7 NaH
SOL 109-99-9 THF

STAGE(2)

RCT BX 79271-56-0
SOL 109-99-9 THF

STAGE(3)

RGT AM 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO BY 412943-04-5, BZ 412943-32-9

RX(22) RCT BY 412943-04-5, S 37595-74-7
RGT U 40949-94-8 K [N(SiMe3)2]
PRO CB 412943-05-6
SOL 109-99-9 THF, 108-88-3 PhMe

RX(23) RCT AI 630-08-0

STAGE(1)

RGT AL 603-35-0 PPh3
CAT 3375-31-3 Pd(OAc)2
SOL 67-56-1 MeOH, 121-44-8 Et3N

STAGE(2)

RCT CB 412943-05-6
SOL 68-12-2 DMF

STAGE(3)

RGT AM 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO CC 412943-06-7

RX(24) RCT CC 412943-06-7, AG 67-56-1

STAGE(1)

RGT CE 471-34-1 CaCO3, CF 2712-78-9 PhI(O2CCF3)2
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2, 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

Updated Search

10509228

STAGE(3)

RGT O 108-48-5 2,6-Lutidine, BX 79271-56-0 F3CSO3SiEt3
SOL 75-09-2 CH2Cl2

STAGE(4)

RGT AG 67-56-1 MeOH

PRO CD 412943-07-8

RX(25) RCT CD 412943-07-8

STAGE(1)

RGT AQ 1191-15-7 AlH(Bu-i)2
SOL 108-88-3 PhMe

STAGE(2)

RGT AG 67-56-1 MeOH

PRO CH 241819-19-2

RX(26) RCT CH 241819-19-2
RGT AT 75-91-2 t-BuOOH
PRO CI 241819-46-5
CAT 3153-26-2 VO acetylacetonate
SOL 71-43-2 Benzene, 124-18-5 Decane

RX(27) RCT CI 241819-46-5, AY 5804-85-3
PRO CJ 412943-08-9
SOL 108-88-3 PhMe

RX(28) RCT CJ 412943-08-9

STAGE(1)

RGT AB 124-63-0 MeSO2Cl, AC 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)

RGT AD 584-08-7 K2CO3
SOL 67-56-1 MeOH

STAGE(3)

RGT AE 7782-44-7 O2
SOL 60-29-7 Et2O

STAGE(4)

RGT AF 144-62-7 (CO2H)2

PRO K 241819-21-6
NTE other product(s) also detected

RX(3) RCT K 241819-21-6

STAGE(1)

SOL 64-19-7 AcOH, 7732-18-5 Water

STAGE(2)

RGT N 77-76-9 Me2C(OMe)2
CAT 3144-16-9 10-CSA
SOL 75-09-2 CH2Cl2

Updated Search

10509228

STAGE(3)

RCT L 69739-34-0
RGT O 108-48-5 2,6-Lutidine

STAGE(4)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO M 241819-23-8

RX(36) RCT M 241819-23-8

STAGE(1)

RGT CL 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DA 241819-24-9

RX(37) RCT DA 241819-24-9
RGT BG 20039-37-6 PDC
PRO H 241819-25-0
SOL 75-09-2 CH2Cl2

RX(2) RCT H 241819-25-0
PRO I 241819-26-1
SOL 64-19-7 AcOH, 7732-18-5 Water

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

Updated Search

10509228

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4
PhI(OAc)2
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT D 75-75-2 MeSO3H
SOL 67-66-3 CHCl3

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO3
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

L3 ANSWER 28 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 136:5852 CASREACT

TITLE: New process for the preparation of vinyl-pyrrolidinone
cephalosporin derivatives

INVENTOR(S): Hebeisen, Paul; Hilpert, Hans; Humm, Roland

PATENT ASSIGNEE(S): Basilea Pharmaceutica A.-G., Switz.

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090111	A1	20011129	WO 2001-EP5721	20010518
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002019381	A1	20020214	US 2001-860157	20010517

Updated Search

10509228

US 6504025	B2	20030107		
CA 2408941	AA	20011129	CA 2001-2408941	20010518
EP 1289998	A1	20030312	EP 2001-936374	20010518
EP 1289998	B1	20050330		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003535059	T2	20031125	JP 2001-586298	20010518
EP 1435357	A2	20040707	EP 2004-2120	20010518
EP 1435357	A3	20060503		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
CN 1603327	A	20050406	CN 2004-10070031	20010518
AT 292135	E	20050415	AT 2001-936374	20010518
PT 1289998	T	20050630	PT 2001-936374	20010518
ES 2238441	T3	20050901	ES 2001-1936374	20010518

PRIORITY APPLN. INFO.:

EP 2000-111164	20000524
CN 2001-809931	20010518
EP 2001-936374	20010518
WO 2001-EP5721	20010518

OTHER SOURCE(S): MARPAT 136:5852
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

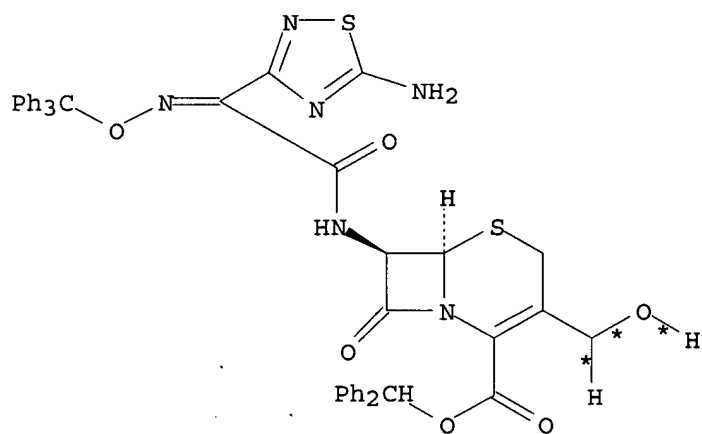
AB A process for preparing pharmaceutical compns., a vinyl-pyrrolidinone cephalosporin derivative of I via the acylation of deacetyl-7-aminocephalosporanic acid with II (R1 = a hydroxy protecting group; Y1-Y3 = an activating group) in base followed by the protection of the carboxylic acid group, formation of an aldehyde at C3 using an inorg. hypohalite in TEMPO or with MnO2, and reacting the aldehyde with III (R = an amino protecting group or group A), was accomplished. I can be used for the treatment and prophylaxis of infectious diseases, especially infectious diseases caused by bacterial pathogens in particular methicillin resistant Staphylococcus aureus (MRSA) and Pseudomonas aeruginosa (no data).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 29 ...D ==> G...

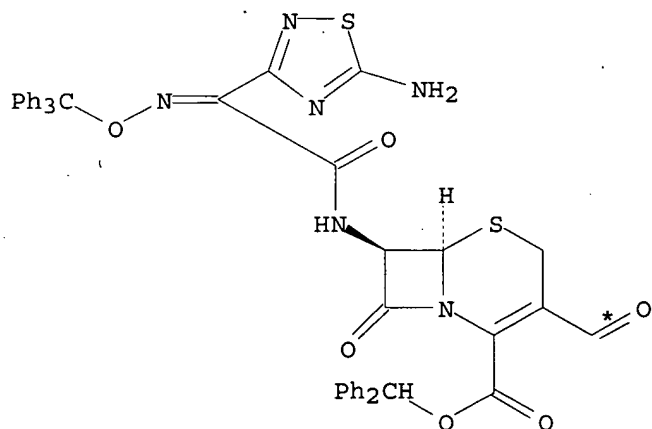
Updated Search

10509228



D

(2) →



G

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO₃, J 2564-83-2

Me₄-piperidoxyl

SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

STAGE(2)

RGT K 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO G 376653-37-1

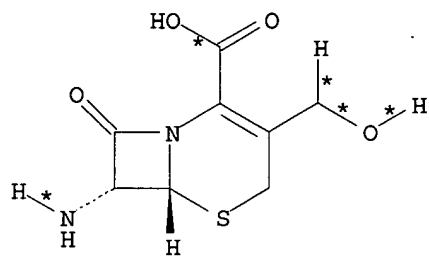
NTE alternative prepn. shown

RX(9) OF 29 COMPOSED OF RX(1), RX(2)

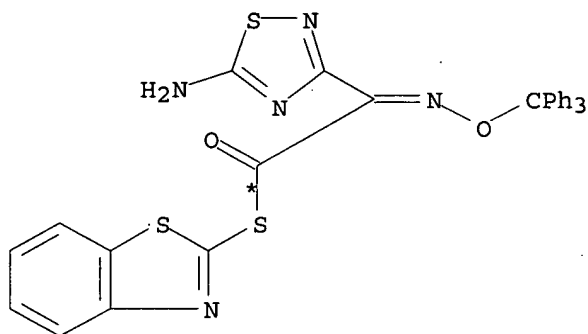
RX(9) A + B + C ==> G

Updated Search

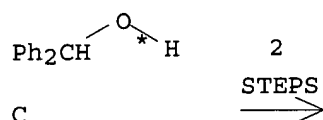
10509228



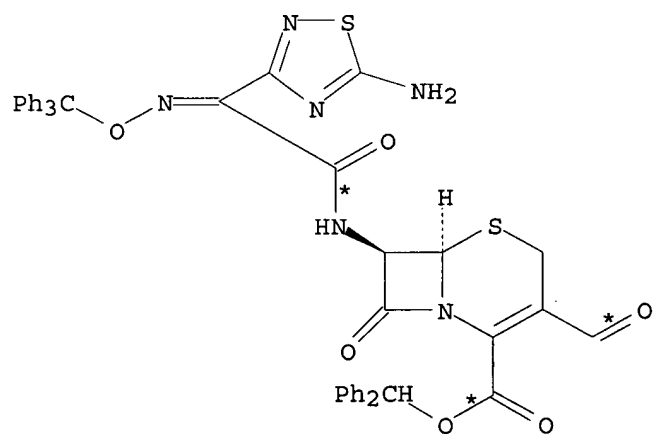
A



B



C



G

RX(1) RCT A 15690-38-7

STAGE(1)

RGT E 80-70-6 Me2NC(:NH)NMe2

SOL 68-12-2 DMF

STAGE(2)

RCT B 209467-59-4, C 91-01-0

PRO D 376653-36-0

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO3, J 2564-83-2

Updated Search

10509228

Me4-piperidoxyl
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

STAGE(2)

RGT K 7681-52-9 NaOCl
SOL 7732-18-5 Water

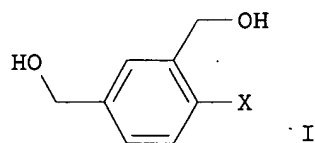
PRO G 376653-37-1
NTE alternative prepn. shown

L3 ANSWER 29 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134:326394 CASREACT
TITLE: Preparation of citalopram intermediates.
INVENTOR(S): Ikemoto, Tetsuya; Igi, Masami
PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1095926	A2	20010502	EP 2000-118562	20000826
EP 1095926	A3	20030507		
EP 1095926	B1	20041006		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6310222	B1	20011030	US 2000-648048	20000825
AT 278654	E	20041015	AT 2000-118562	20000826
PT 1095926	T	20041231	PT 2000-118562	20000826
ES 2228369	T3	20050416	ES 2000-118562	20000826
CA 2317002	AA	20010501	CA 2000-2317002	20000829
AU 2000055008	A5	20010503	AU 2000-55008	20000830
AU 781464	B2	20050526		
JP 2002121161	A2	20020423	JP 2000-285068	20000920
JP 3641420	B2	20050420		
US 2001056194	A1	20011227	US 2001-909596	20010720
US 6395910	B2	20020528		
US 2002045770	A1	20020418	US 2001-997992	20011130
US 6433195	B2	20020813		
US 2002151728	A1	20021017	US 2002-176721	20020621
US 2004044232	A1	20040304	US 2003-650876	20030828
US 6930211	B2	20050816		
US 2005080278	A1	20050414	US 2003-650875	20030828
US 2006167285	A1	20060727	US 2006-386018	20060321
PRIORITY APPLN. INFO.:			JP 1999-311703	19991101
			JP 2000-245427	20000811
			US 2000-648048	20000825
			US 2001-909596	20010720
			US 2001-997992	20011130
			US 2002-176721	20020621
			US 2003-650875	20030828
OTHER SOURCE(S):	MARPAT 134:326394			
GI				

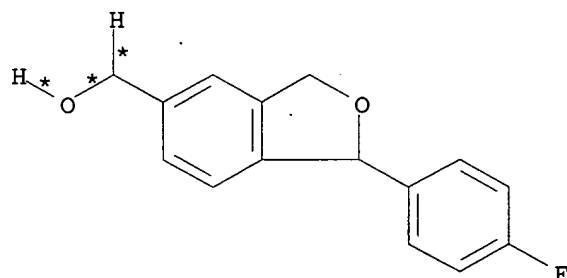
Updated Search

10509228

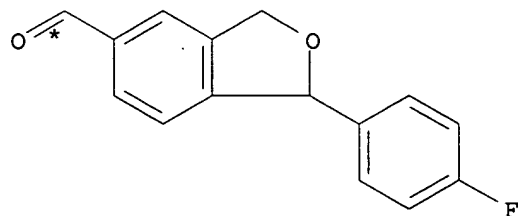


AB Title compds., e.g., (I; X = Cl, Br, iodo), were prepared Thus, 2,4-bis(acetoxymethyl)bromobenzene (preparation given) in MeOH at 10° was treated with aqueous NaOH, stirred for 1 h, and solvent was evaporated The residue was neutralized with aqueous HCl followed by addition of PhMe and heating to 80-85° for 1 h to give 83.7% 2,4-bis(hydroxymethyl)bromobenzene. This was stirred with Et vinyl ether and p-toluenesulfonic acid in PhMe followed by 2 h stirring to give 97.1% 2,4-bis(1-ethoxyethoxymethyl)bromobenzene. The latter in THF at -40° was treated with BuLi followed by warming to -20°, treatment with p-fluorobenzaldehyde, and warming to 15° over 1 h to give 88.7% 1-(4-fluorophenyl)-1,3-dihydrobenzofuran-5-ylmethanol, which was converted to 1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile in 3 steps.

RX(6) OF 28U ==> Z...



(6) →



YIELD 84%

RX(6) RCT U 335612-71-0

Updated Search

STAGE(1)

RGT AA 144-55-8 NaHCO₃, AB 1643-19-2 Bu₄N.Br, AC
2564-83-2 Me₄-piperidoxyl
SOL 141-78-6 AcOEt

STAGE(2)

RGT AD 7681-52-9 NaOCl
SOL 7732-18-5 Water

STAGE(3)

SOL 7732-18-5 Water

PRO Z 335612-72-1

L3 ANSWER 30 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:115518 CASREACT

TITLE: A New Polymer-Attached Reagent for the Oxidation of
Primary and Secondary Alcohols

AUTHOR(S): Sourkouni-Argirusi, Georgia; Kirschning, Andreas

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet
Hannover, Hannover, D-30167, Germany

SOURCE: Organic Letters (2000), 2(24), 3781-3784

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

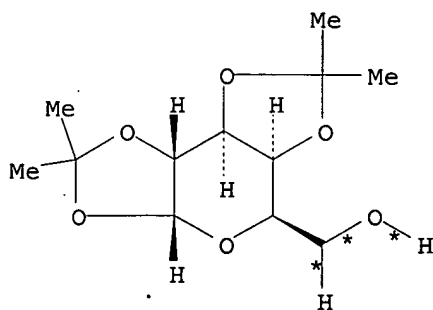
DOCUMENT TYPE: Journal

LANGUAGE: English

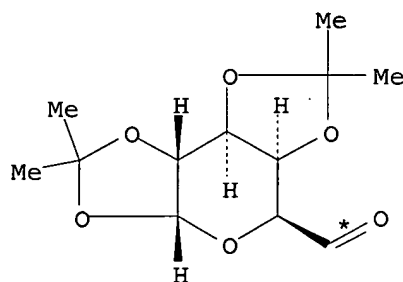
AB A new, polymer-bound reagent system for the efficient oxidation of primary alcs. to aldehydes and secondary alcs. to ketones in the presence of a catalytic amount of 2,2,6,6-tetramethyl-1-piperidinyloxyl (TEMPO) is described. The reagent was prepared by treating a com. available polymer-bound bromide (Fluka) with bis(acetato-κO)phenyliodine to give a polymer-bound trimethylammonium-bis(acetato-κO)bromate(1-) reagent. In most cases, workup of this heavy metal-free oxidation is achieved by simple filtration followed by removal of the solvent. In selected examples this reagent was compared with the known polymer-bound permanganate and chromium(VI) reagents.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(11) OF 18 AC ==> AD



AC

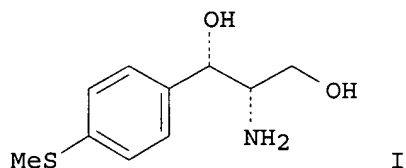


AD
YIELD 97%

10509228

RX(11) RCT AC 4064-06-6
RGT D 74-89-5D MeNH₂, J 2564-83-2 Me₄-piperidoxyl
PRO AD 4933-77-1
SOL 75-09-2 CH₂Cl₂
NTE STEREOSELECTIVE

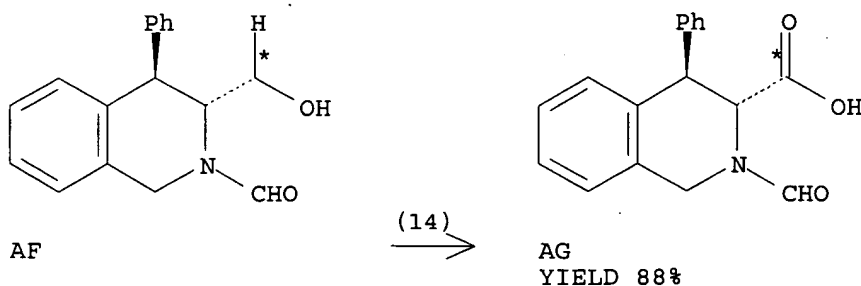
L3 ANSWER 31 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 133:296358 CASREACT
TITLE: Stereoselective synthesis of 3-mono- and
1,3-disubstituted 4-phenyl-1,2,3,4-
tetrahydroisoquinolines
AUTHOR(S): Brozda, D.; Koroniak, L.; Rozwadowska, M. D.
CORPORATE SOURCE: Grunwaldzka 6, Faculty of Chemistry, Adam Mickiewicz
University, Poznan, 60-780, Pol.
SOURCE: Tetrahedron: Asymmetry (2000), 11(14), 3017-3025
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB (1S,2S)-(+)-Thiomicamine I was transformed in high yield and with high diastereoselectivity into (3R,4R)-4-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid and enantiomerically pure (3R,4R)-3-hydroxymethyl-4-phenyl- and (1R,3R,4R)-3-hydroxymethyl-1-methyl-4-phenyl-1,2,3,4-tetrahydroisoquinoline derivs.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(14) OF 52 ...AF ==> AG...



RX(14) RCT AF 294869-50-4

Updated Search

10509228

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO3,
AJ 7758-02-3 KBr, AK 1112-67-0 Bu4NCl
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO3, AM 7647-14-5 NaCl
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

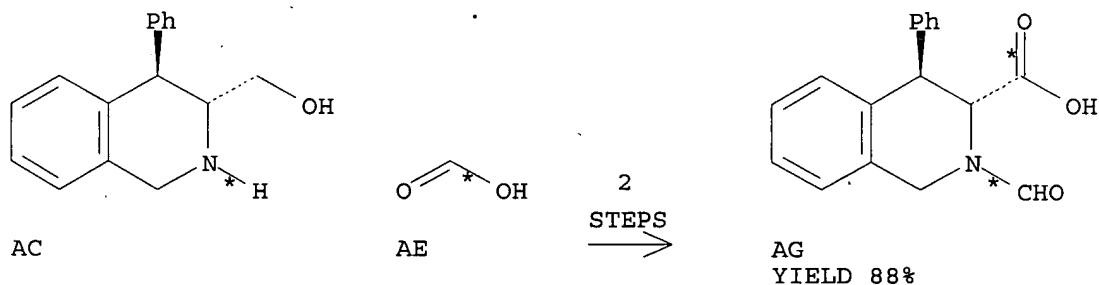
STAGE(5)

SOL 75-09-2 CH2Cl2

PRO AG 294869-51-5
NTE STEREOSELECTIVE

RX(30) OF 52 COMPOSED OF RX(13), RX(14)

RX(30) AC + AE ==> AG



RX(13) RCT AC 300698-53-7, AE 64-18-6
PRO AF 294869-50-4
SOL 108-88-3 PhMe
NTE STEREOSELECTIVE

RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO3,
AJ 7758-02-3 KBr, AK 1112-67-0 Bu4NCl
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO3, AM 7647-14-5 NaCl
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

Updated Search

10509228

STAGE(5)

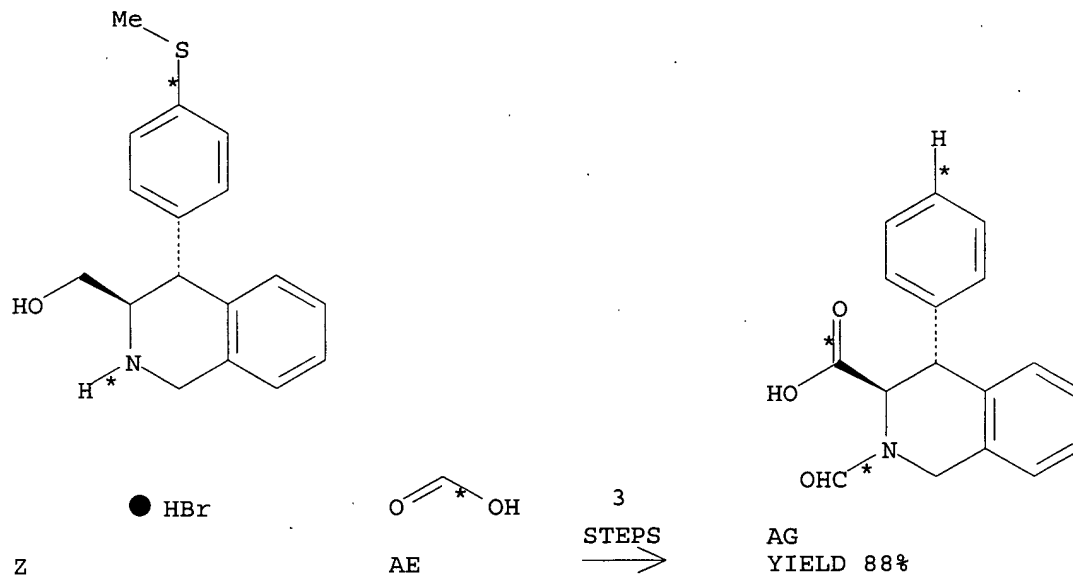
SOL 75-09-2 CH₂Cl₂

PRO AG 294869-51-5

NTE STEREOSELECTIVE

RX(42) OF 52 COMPOSED OF RX(11), RX(13), RX(14)

RX(42) Z + AE ==> AG



RX(11) RCT Z 294869-46-8

STAGE(1)

RGT P 7647-01-0 HCl

SOL 109-99-9 THF

STAGE(2)

RGT AD 7440-02-0 Ni

PRO AC 300698-53-7

NTE STEREOSELECTIVE

RX(13) RCT AC 300698-53-7, AE 64-18-6

PRO AF 294869-50-4

SOL 108-88-3 PhMe

NTE STEREOSELECTIVE

RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me₄-piperidoxyl, AI 144-55-8 NaHCO₃,

AJ 7758-02-3 KBr, AK 1112-67-0 Bu₄NCl

SOL 75-09-2 CH₂Cl₂

Updated Search

10509228

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO₃, AM 7647-14-5 NaCl
SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

STAGE(5)

SOL 75-09-2 CH₂Cl₂

PRO AG 294869-51-5
NTE STEREOSELECTIVE

L3 ANSWER 32 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 127:65794 CASREACT

TITLE: Oxidation of primary or secondary alcohols using
N-chloro compounds and piperidinyloxy derivatives.

INVENTOR(S): Jenny, Christian-Johannes; Lohri, Bruno; Schlageter,
Markus

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

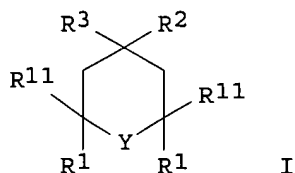
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 775684	A1	19970528	EP 1996-118157	19961113
EP 775684	B1	19990818		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
US 5821374	A	19981013	US 1996-747944	19961112
CN 1156713	A	19970813	CN 1996-114464	19961113
CN 1073074	B	20011017		
AT 183492	E	19990915	AT 1996-118157	19961113
ES 2136930	T3	19991201	ES 1996-118157	19961113
JP 09169685	A2	19970630	JP 1996-304291	19961115
			CH 1995-3291	19951121

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 127:65794

GI



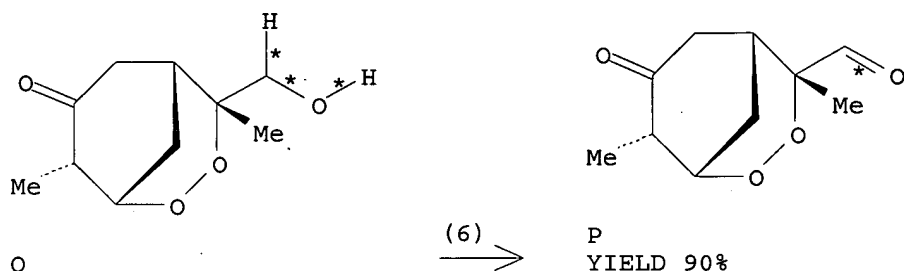
AB Primary and secondary alcs. are oxidized using organic N-chloro compds. in the presence of cyclic amine derivs (I; R₁, R₁₁ = alkyl; R₂, R₃ = H, alkoxy, OH, alkylcarbonyloxy, arylcarbonyloxy, alkylcarbonylamino; R₂R₃ =

Updated Search

10509228

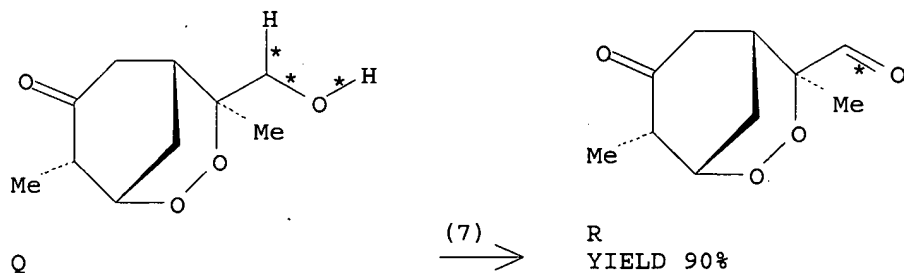
ketal group; Y = N+:O X-, NOH, NO·; X- = anion). Thus, a mixture of (1S,4R,5R,8S)-4-hydroxymethyl-4,8-dimethyl-2,3-dioxabicyclo[3.3.1]nonane-7-one 46.2% and (1S,4S,5R,8S)-4-hydroxymethyl-4,8-dimethyl-2,3-dioxabicyclo[3.3.1]nonane-7-one 47.5% together with NaOAc and trichloroisocyanuric acid in CH₂Cl₂ at 0° was treated with TEMPO in CH₂Cl₂ and the mixture was stirred 5 h at 0-3° to give >90% crude yield of (1S,4R,5R,8S)-4,8-dimethyl-7-oxo-2,3-dioxabicyclo[3.3.1]nonane-4-carboxaldehyde 42.3% and (1S,4S,5R,8S)-4,8-dimethyl-7-oxo-2,3-dioxabicyclo[3.3.1]nonane-4-carboxaldehyde 45.8%.

RX(6) OF 7 O ==> P



RX(6) RCT O 160420-93-9
RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2
Me4-piperidoxyl, E 127-09-3 AcONa
PRO P 160497-32-5
SOL 75-09-2 CH₂Cl₂

RX(7) OF 7 Q ==> R



RX(7) RCT Q 191406-57-2
RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2
Me4-piperidoxyl, E 127-09-3 AcONa
PRO R 160497-33-6
SOL 75-09-2 CH₂Cl₂

L3 ANSWER 33 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 123:9432 CASREACT
TITLE: Method of preparing enantiomerically pure

Updated Search

10509228

INVENTOR(S): 3-methyl-5-[1-alkyl-2(S)-pyrrolidinyl]isoxazoles
 Lin, Nan-Horng; He, Yun; Elliott, Richard L.;
 Chorghade, Mukund S.; Wittenberger, Steven J.;
 Bunnelle, William H.; Narayanan, Bikshandar A.;
 Singam, Pulla R.; Esch, Thomas K. J.; et al.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 41 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

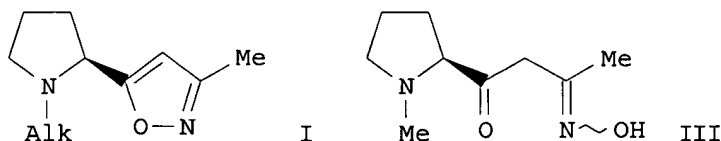
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9507277	A1	19950316	WO 1994-US9734	19940830
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5424444	A	19950613	US 1994-234442	19940428
EP 717741	A1	19960626	EP 1994-931741	19940830
EP 717741	B1	20010530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09502439	T2	19970311	JP 1994-508711	19940830
GR 3036387	T3	20011130	GR 2001-401243	20010814
PRIORITY APPLN. INFO.:			US 1993-117819	19930908
			US 1994-234442	19940428
			US 1992-981587	19921125
			WO 1994-US9734	19940830

OTHER SOURCE(S): MARPAT 123:9432

GI

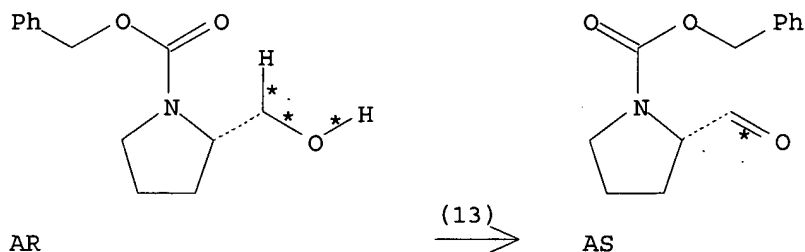


AB Several novel processes for preparing enantiomerically pure title compds. I [Alk = C1-3 alkyl] in high yield are described. I are known cholinergic ligands with selectivity for neuronal nicotinic receptors (no data). In the new methods, a protected pyrrolidine or 2-oxopyrrolidine starting material reacts with a suitable organic anion, and a resulting β -keto oxime intermediate is cyclized and dehydrated. For example, L-proline reacted with SO_2Cl_2 in MeOH, followed by $\text{HC}(\text{OMe})_3$, to give the Me ester hydrochloride, which was reductively methylated with aqueous H_2CO and H_2 over Pd/C to give N-methylproline Me ester (II). Acetone oxime was converted by BuLi in THF to its dianion, which reacted with II to give dione oxime III. Cyclization of III by mesyl chloride and Et_3N in CH_2Cl_2 gave I [Alk = Me]. Addnl. preps. are described, on small, intermediate, and large (15 kg) scale.

RX(13) OF 84 ...AR ==> AS...

Updated Search

10509228



RX(13) RCT AR 6216-63-3

STAGE(1)

RGT AT 7647-15-6 NaBr

SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)

RGT AU 2564-83-2 Me4-piperidoxyl

STAGE(3)

RGT G 497-19-8 Na₂CO₃, AV 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO AS 71461-30-8

L3 ANSWER 34 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 116:20658 CASREACT

TITLE: A general synthetic method for the oxidation of primary alcohols to aldehydes: (S)-(+)-2-methylbutanal

AUTHOR(S): Anelli, Pier Lucio; Montanari, Fernando; Quici, Silvio

CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milan, I-20133, Italy

SOURCE: Organic Syntheses (1990), 69, 212-19

CODEN: ORSYAT; ISSN: 0078-6209

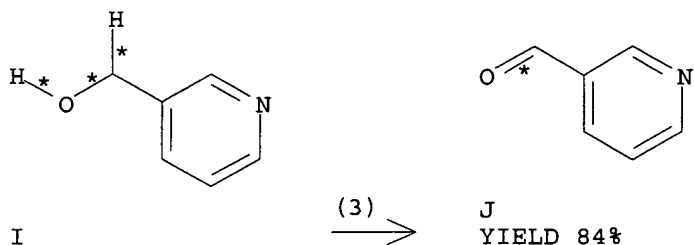
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rapid, inexpensive, selective oxidation of alcs. to aldehydes was achieved by the oxidation of alcs. with sodium hypochlorite in the presence of 2,2,6,6-tetramethylpiperidin-1-oxyl and KBr. The oxidation of (S)-2-methyl-1-butanol with sodium hypochlorite in the presence of 2,2,6,6-tetramethylpiperidin-1-oxyl and KBr gave 82-84% (S)-2-methylbutanal.

RX(3) OF 4 I ==> J

10509228



RX(3) RCT I 100-55-0
RGT C 7681-52-9 NaOCl, D 2564-83-2 Me4-piperidoxyl, E
7758-02-3 KBr
PRO J 500-22-1
SOL 75-09-2 CH2Cl2

L3 ANSWER 35 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 115:231347 CASREACT

TITLE: Organic oxoammonium salts. 3. A new convenient method for the oxidation of alcohols to aldehydes and ketones

AUTHOR(S): Ma, Zhenkun; Bobbitt, James M.

CORPORATE SOURCE: Dep. Chem., Univ. Connecticut, Storrs, CT, 06269-3060, USA

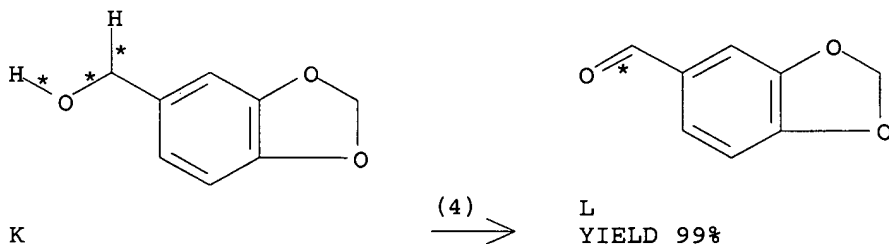
SOURCE: Journal of Organic Chemistry (1991), 56(21), 6110-14
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new method for the selective oxidation of alcs. using organic oxo ammonium salts generated by acid-promoted disproportionation of nitroxides (e.g., 4-acetylamino-2,2,6,6-tetramethylpiperidiny1-1-oxyl) in solution were developed. Major advantages are high yields, ease of product isolation, and a high degree of selectivity in the presence of other functional groups.

RX(4) OF 4 K ==> L

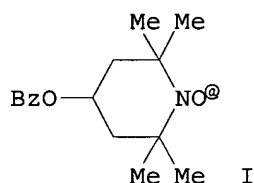


RX(4) RCT K 495-76-1
RGT C 14691-89-5 1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-, D 104-15-4 TsOH
PRO L 120-57-0
SOL 75-09-2 CH2Cl2

Updated Search

10509228

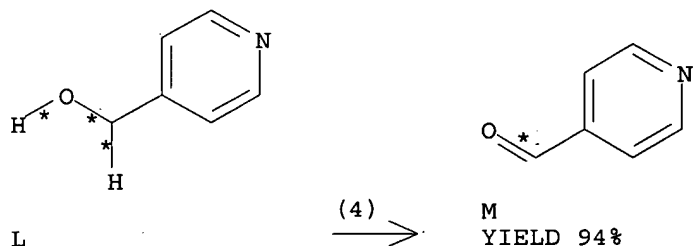
L3 ANSWER 36 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 115:113733 CASREACT
TITLE: A new oxidizing system for aromatic alcohols by the
combination of N-oxoammonium salt and
electrosynthesized tetraalkylammonium tribromide
AUTHOR(S): Inokuchi, Tsutomu; Matsumoto, Sigeaki; Fukushima,
Mitsuhiro; Torii, Sigeru
CORPORATE SOURCE: Fac. Eng., Okayama Univ., Okayama, 700, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1991),
64(3), 796-800
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB A combination of piperidinyloxyl I and tetraalkylammonium tribromides (R₄NBr₃), which are available from the corresponding tetraalkylammonium bromides via electrooxidn. with KBr, is useful for oxidation of primary and secondary alcs. to aldehydes and ketones, resp. The oxidation proceeds smoothly even with 0.5-1.0 mol % I and 1.5-2.0 equiv of tetraalkylammonium tribromide in an aqueous-organic two-phase solution buffered at pH 8.0-8.6.

This recyclable oxidant/cooxidant system may involve formation of N-oxoammonium salts, the actual oxidizing agents of alcs., by the action of hypobromite species generated from R₄NBr₃ in the binary solution. Benzylic alcs. bearing electron-releasing groups on the aromatic nucleus are oxidized to aldehydes or ketones without any bromination and overoxidn.

RX(4) OF 4 L ==> M



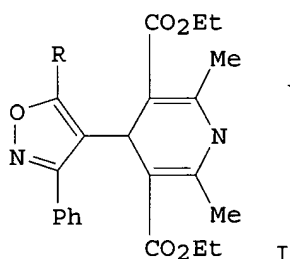
RX(4) RCT L 586-95-8
RGT C 3225-26-1 Piperidinoxy deriv., D 38932-80-8
Bu₄N.Br₃, E 127-09-3 AcONa
PRO M 872-85-5

Updated Search

10509228

RX(12) RCT AC 123903-23-1
RGT D 3225-26-1 Piperidinooxy deriv., E 7486-26-2 NaBrO2,
C 144-55-8 NaHCO3
PRO AD 123903-24-2
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

L3 ANSWER 38 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 108:55850 CASREACT
TITLE: Cardioactivity and solid-state structure of two
4-isoxazolyldihydropyridines related to the
4-aryldihydropyridine calcium-channel blockers
AUTHOR(S): McKenna, John I.; Schlicksupp, Ludwig; Natale,
Nicholas R.; Willett, Roger D.; Maryanoff, Bruce E.;
Flaim, Stephen F.
CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, 83843, USA
SOURCE: Journal of Medicinal Chemistry (1988), 31(2), 473-6
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

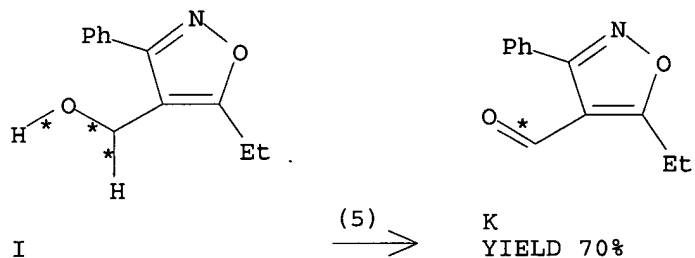


AB Di-Et 2,6-dimethyl-4-(5-ethyl-3-phenyl-4-isoxazolyl)-1,4-dihydropyridine-3,5-dicarboxylate (I, R = Et) and di-Et 2,6-dimethyl-4-(5-isopropyl-3-phenyl-4-isoxazolyl)-1,4-dihydropyridine-3,5-dicarboxylate (I, R = Me2CH) were prepared by Hantzsch cyclization of the isoxazolyl aldehydes with EtO2CCH2Ac and NH3. The mol. structures of I were determined by x-ray crystallog. In I (R = Et), which has an Et group at the C5 position of the isoxazole ring, the deviation from planarity in the dihydropyridine (DHP) ring is the smallest of all known DHP derivs. The dihedral angle between the isoxazole ring and the DHP ring, which is approx. 90° in similar biol. active dihydropyridines, is somewhat smaller (82.7° and 85.2°, resp.) in these two compds. In both compds., one of the ester groups is coplanar with the DHP ring while the other one is out of plane by 14.7° (R = Et) and 18.8° (R = Me2CH). Both I were found to be vasodilators in the Langendorff assay. The potency of I (R = Me2CH) on cardiac flow was similar to that of nifedipine; however, that of I (R = Et) was considerably attenuated. Since isoxazolyl analog I (R = Me2CH) lacks the significant neg. inotropic activity associated with nifedipine, it offers promise as an antihypertensive or antianginal agent.

RX(5) OF 24 ...I ==> K...

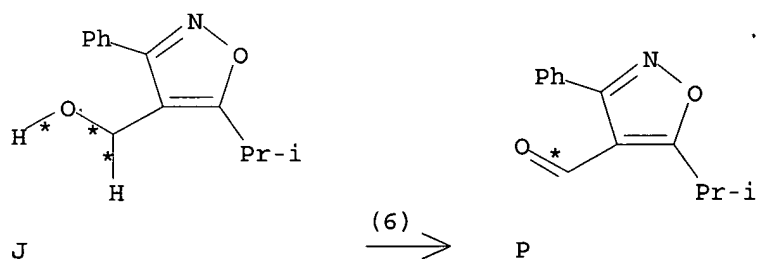
Updated Search

10509228



RX(5) RCT I 99299-07-7
RGT L 7782-44-7 O2, M 2564-83-2 Me4-piperidoxyl
PRO K 99298-93-8
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF

RX(6) OF 24 ...J ==> P...



RX(6) RCT J 99299-09-9
RGT L 7782-44-7 O2, M 2564-83-2 Me4-piperidoxyl
PRO P 111525-13-4
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF

=> d his

(FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006)

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

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L2 3 S L1
L3 38 S L1 FULL
L4 0 S L3 AND SHIOMI, Y?/AU
L5 0 S L3 AND UNO, O?/AU
L6 0 S L3 AND OHTA, A?/AU
L7 0 S L3 AND SUNAKAMI, T?/AU

=> FIL REGISTRY

COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
371.88	372.09

Updated Search

10509228

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CA SUBSCRIBER PRICE	-26.98	-26.98

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DICTIONARY FILE UPDATES: 11 OCT 2006 HIGHEST RN 910211-10-8

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=> S 7782-44-7/RN

L8 1 7782-44-7/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L8 SQIDE .1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 7782-44-7 REGISTRY
CN Oxygen (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Dioxygen
CN Molecular oxygen
CN Oxygen molecule
DR 1338-93-8, 14797-70-7, 80217-98-7, 80937-33-3
MF O2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA,

Updated Search

10509228

MEDLINE, MRCK*, MSDS-OHS, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER,
TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

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DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent;
Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC
(Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);
PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role
in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical
study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC
(Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);
PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological
study); CMBI (Combinatorial study); FORM (Formation, nonpreparative);
MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC
(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses);
NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
study); BIOL (Biological study); CMBI (Combinatorial study); FORM
(Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence);
PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or
reagent); USES (Uses)

O—O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

390743 REFERENCES IN FILE CA (1907 TO DATE)

36372 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

391458 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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NOTICE SET TO OFF FOR DISPLAY COMMAND
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=> d his

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FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

L1 STRUCTURE UPLOADED
L2 3 S L1
L3 38 S L1 FULL
L4 0 S L3 AND SHIOMI, Y?/AU
L5 0 S L3 AND UNO, O?/AU
L6 0 S L3 AND OHTA, A?/AU
L7 0 S L3 AND SUNAKAMI, T?/AU

Updated Search

10509228

FILE 'REGISTRY' ENTERED AT 19:58:36 ON 12 OCT 2006
L8 1 S 7782-44-7/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

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COST IN U.S. DOLLARS

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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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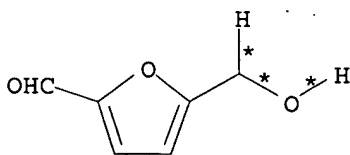
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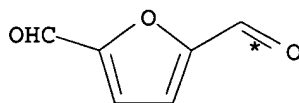
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L3 ANSWER 1 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(2) OF 2 A ==> D



A



D
YIELD 87%

RX(2) RCT A 67-47-0

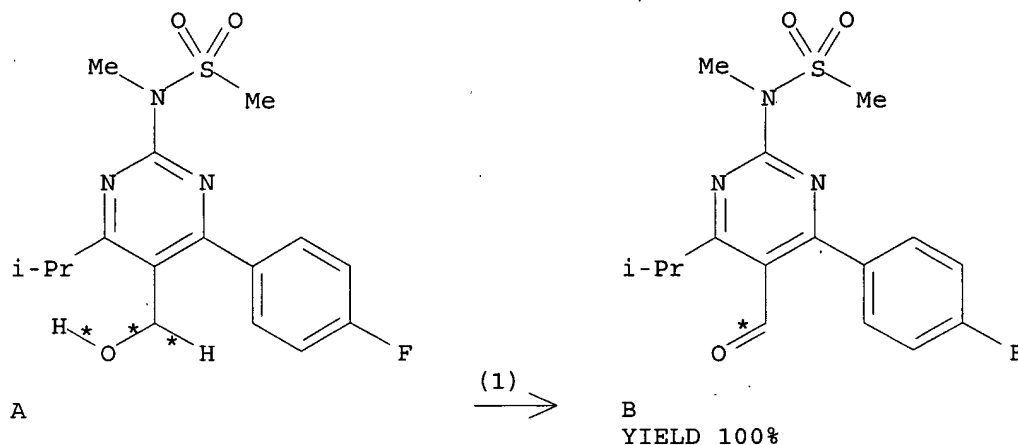
Updated Search

10509228

RGT E 2564-83-2 Me4-piperidoxyl, F 3240-34-4 PhI(OAc)2
PRO D 823-82-5
SOL 108-10-1 i-BuCOMe
CON 1.5 hours, room temperature
NTE optimization study

L3 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

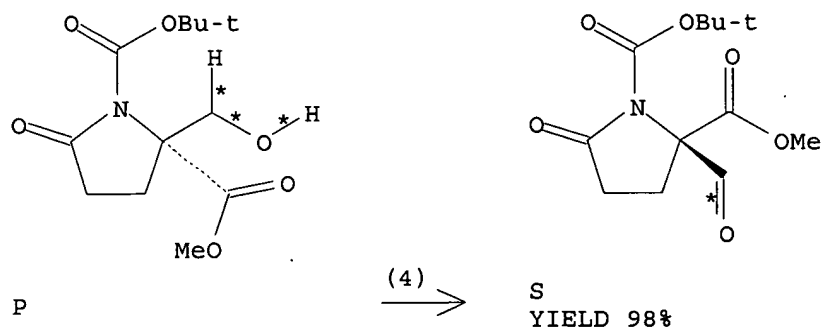
RX(1) OF 11 A ==> B



RX(1) RCT A 147118-36-3
RGT C 2564-83-2 Me4-piperidoxyl, D 7681-52-9 NaOCl, E 7758-02-3 KBr
PRO B 147118-37-4
SOL 7732-18-5 Water, 75-05-8 MeCN
CON SUBSTAGE(1) 5 deg C
SUBSTAGE(3) 6 hours
NTE optimization study

L3 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(4) OF 464 ...P ==> S...



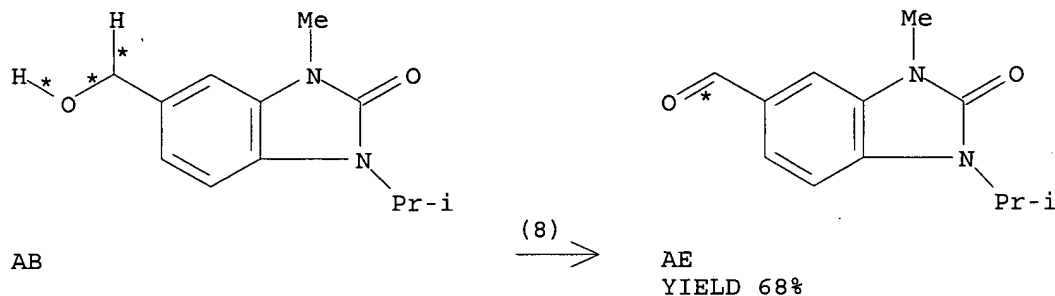
Updated Search

10509228

RX(4) RCT P 866331-68-2
RGT T 2564-83-2 Me4-piperidoxyl, U 3240-34-4 PhI(OAc)2
PRO S 866331-49-9
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 26 hours, room temperature

L3 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

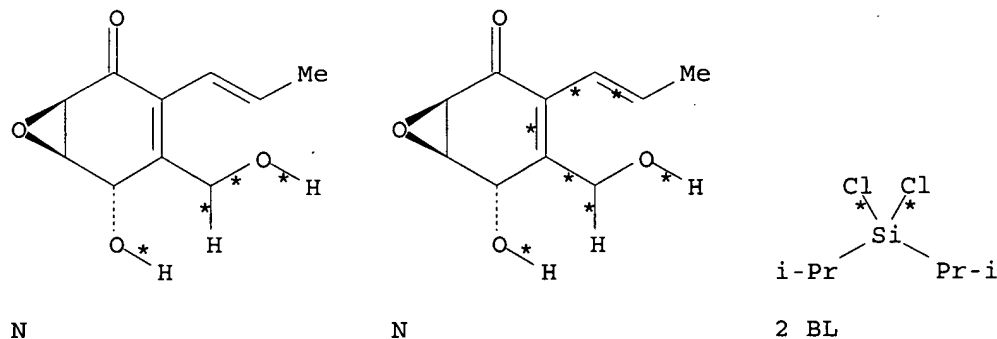
RX(8) OF 71 ...AB ==> AE...



RX(8) RCT AB 865443-84-1
RGT AF 2564-83-2 Me4-piperidoxyl, AG 128-09-6
Chlorosuccinimide, AH 1112-67-0 Bu4NCl
PRO AE 865443-86-3
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 18 hours, 22 deg C, pH 8.6
NTE buffered solution, sodium bicarbonate-potassium carbonate

L3 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

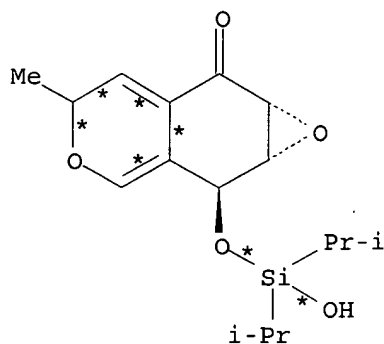
RX(25) OF 255 ...2 N + 2 BL ==> BM + BN...



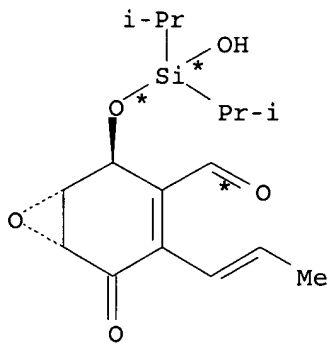
(25)
 \rightarrow

Updated Search

10509228



BM
YIELD 76%



BN
YIELD 15%

RX(25) RCT N 238424-94-7

STAGE(1)

RGT W 2564-83-2 Me4-piperidoxyl, X 7782-44-7 O2, Y
7758-89-6 CuCl
SOL 68-12-2 DMF
CON 1 hour, room temperature, 1 atm

STAGE(2)

RCT BL 7751-38-4
RGT AY 288-32-4 1H-Imidazole
SOL 68-12-2 DMF
CON 15 minutes, 0 deg C

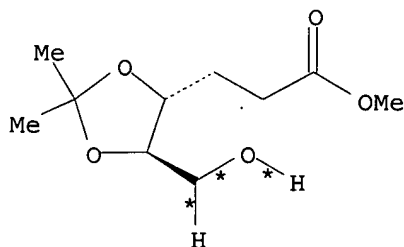
STAGE(3)

RGT L 7732-18-5 Water

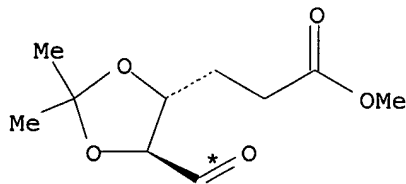
PRO BM 668987-33-5, BN 668987-32-4

L3 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 171 ...AT ==> AX...



AT



AX
YIELD 70%

RX(11) RCT AT 850222-14-9

STAGE(1)

Updated Search

10509228

RGT AY 95407-69-5 1-Piperidinyloxy,
4-methoxy-2,2,6,6-tetramethyl-, AZ 144-55-8 NaHCO₃, BA
7681-52-9 NaOCl, BB 7758-02-3 KBr
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 15 minutes, 0 deg C

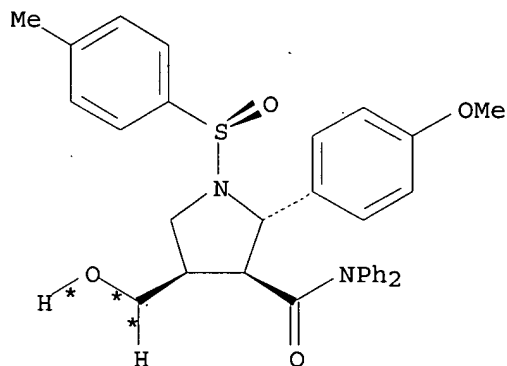
STAGE(2)

RGT O 7772-98-7 Na₂S₂O₃
SOL 7732-18-5 Water

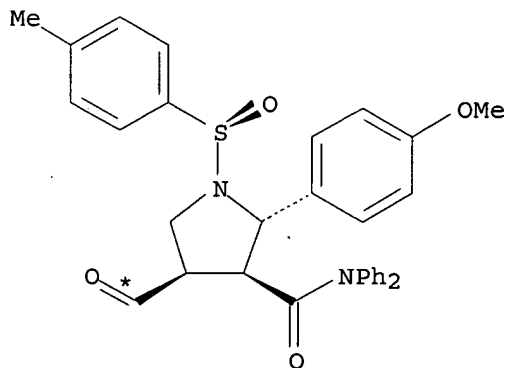
PRO AX 862907-39-9

L3 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 66 ...H ==> L...



H



L

YIELD 91%

RX(3) RCT H 861145-05-3

STAGE(1)

Updated Search

10509228

RGT M 2564-83-2 Me4-piperidoxyl, N 7647-15-6 NaBr
SOL 7732-18-5 Water, 108-88-3 PhMe, 141-78-6 AcOEt
CON room temperature -> 0 deg C

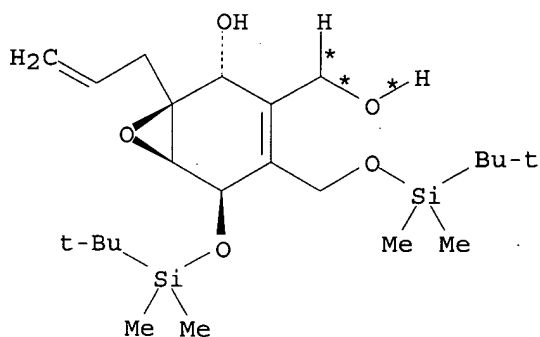
STAGE(2)

RGT O 144-55-8 NaHCO3, P 7681-52-9 NaOCl

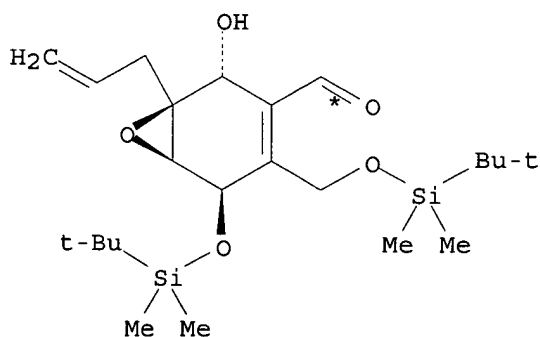
PRO L 861145-06-4

L3 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 105 ...L ==> M...



L



M

YIELD 90%

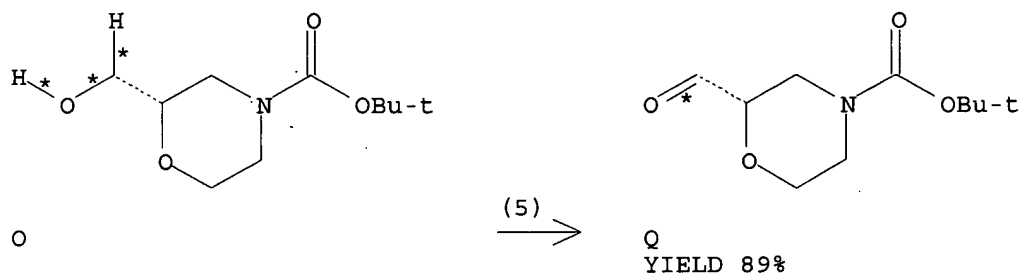
RX(5) RCT L 852392-89-3
RGT N 2564-83-2 Me4-piperidoxyl, O 7782-44-7 O2, P
7758-89-6 CuCl
PRO M 852392-90-6
SOL 68-12-2 DMF
CON 3 hours, room temperature

L3 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

RX(5) OF 81 ...O ==> Q...



RX(5) RCT O 135065-76-8

STAGE(1)

RGT R 2564-83-2 Me4-piperidoxyl, S 144-55-8 NaHCO₃

SOL 141-78-6 AcOEt

CON room temperature -> -5 deg C

STAGE(2)

RGT T 87-90-1 Isocyanuric chloride

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) 1 hour, -5 deg C

SUBSTAGE(2) 1 hour, -5 deg C

STAGE(3)

RGT U 3375-31-3 Pd(OAc)₂

SOL 7732-18-5 Water

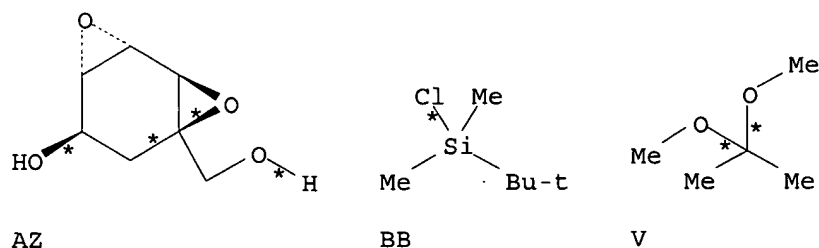
PRO Q 847805-31-6

NTE stereoselective, KEY STEP, Swern oxidn. leads to racemization, use of EtOAc suppresses chlorination

L3 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

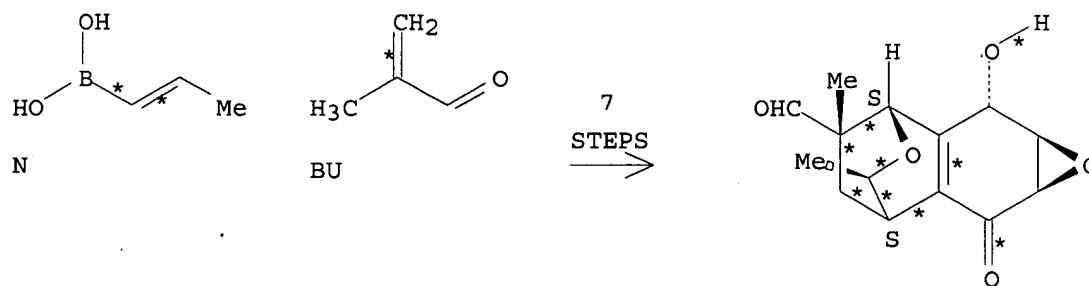
RX(111) OF 236 COMPOSED OF RX(13), RX(5), RX(4), RX(14), RX(3), RX(15), RX(23)

RX(111) AZ + BB + V + N + BU ==> BV



Updated Search

10509228



BV
YIELD 69%

RX(13) RCT AZ 635678-63-6, BB 18162-48-6
RGT BC 121-44-8 Et₃N, BD 1122-58-3 4-DMAP
PRO AA 488808-28-2
SOL 75-09-2 CH₂Cl₂
CON 15 hours, room temperature

RX(5) RCT AA 488808-28-2

STAGE(1)

RGT AB 2564-83-2 Me₄-piperidoxyl, AC 7758-02-3 KBr,
AD 7681-52-9 NaOCl, AE 144-55-8 NaHCO₃
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 40 minutes, -10 deg C, pH 9.5

STAGE(2)

RGT AF 7631-86-9 SiO₂
SOL 108-88-3 PhMe
CON 4.5 hours, 70 deg C

PRO U 488808-29-3

RX(4) RCT U 488808-29-3

STAGE(1)

RGT X 9037-24-5 Amberlyst 15
SOL 67-56-1 MeOH
CON 5 hours, room temperature

STAGE(2)

RCT V 77-76-9
RGT Y 24057-28-1 Pyridinium tosylate
SOL 75-09-2 CH₂Cl₂
CON 4 hours, room temperature

PRO W 488808-30-6

RX(14) RCT W 488808-30-6
RGT AT 7553-56-2 I₂, BE 2712-78-9 PhI(O₂CCF₃)₂, BF 110-86-1 Pyridine
PRO M 488808-31-7
SOL 75-09-2 CH₂Cl₂
CON 22 hours, room temperature
NTE in the dark

Updated Search

10509228

RX(3) RCT M 488808-31-7, N 7547-97-9

STAGE(1)

CAT 14220-64-5 PdCl₂(PhCN)₂, 20667-12-3 Ag₂O, 603-32-7 Ph₃As
SOL 109-99-9 THF, 7732-18-5 Water
CON 11 hours, room temperature

STAGE(2)

RGT P 12125-02-9 NH₄Cl
SOL 7732-18-5 Water
CON 1 hour, room temperature

PRO O 238424-99-2
NTE in the dark

RX(15) RCT O 238424-99-2
RGT X 9037-24-5 Amberlyst 15
PRO G 238424-94-7
SOL 67-56-1 MeOH
CON 40 minutes, room temperature

RX(23) RCT G 238424-94-7

STAGE(1)

RGT K 1313-13-9 MnO₂
SOL 75-09-2 CH₂Cl₂
CON 1 hour, 0 deg C

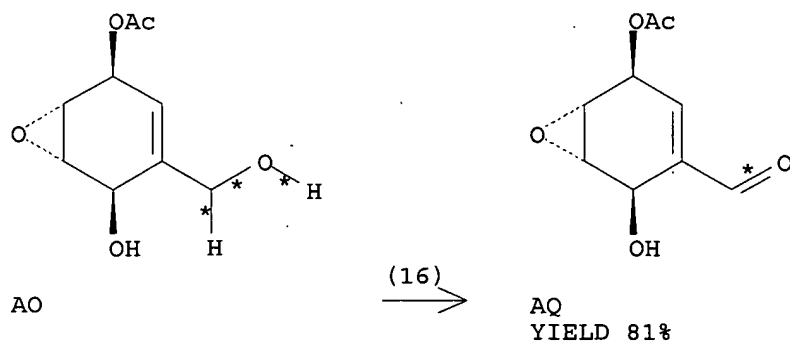
STAGE(2)

RCT BU 78-85-3
CON room temperature

PRO BV 832731-77-8
NTE stereoselective

L3 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(16) OF 185 ...AO ==> AQ...



RX(16) RCT AO 792910-40-8
RGT AR 2564-83-2 Me₄-piperidoxyl, AS 7758-89-6 CuCl, AT
7782-44-7 O₂
PRO AQ 792910-42-0

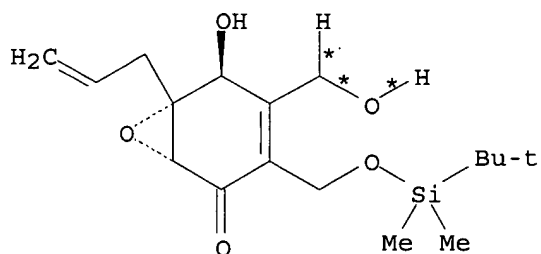
Updated Search

10509228

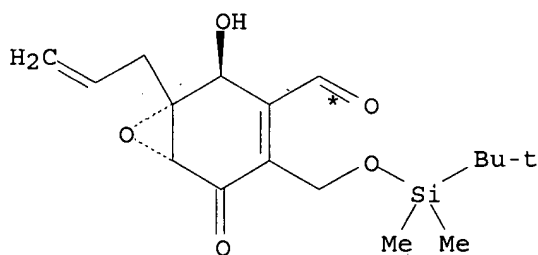
SOL 68-12-2 DMF
CON room temperature

L3 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(9) OF 230 ...Y ==> AA...



Y



AA
YIELD 90%

RX(9) RCT Y 791854-39-2

STAGE(1)

RGT AB 2564-83-2 Me4-piperidoxyl, AC 7681-65-4 CuI
SOL 68-12-2 DMF
CON 3 hours, room temperature

STAGE(2)

RGT AD 7758-98-7 CuSO4
SOL 7732-18-5 Water

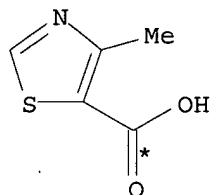
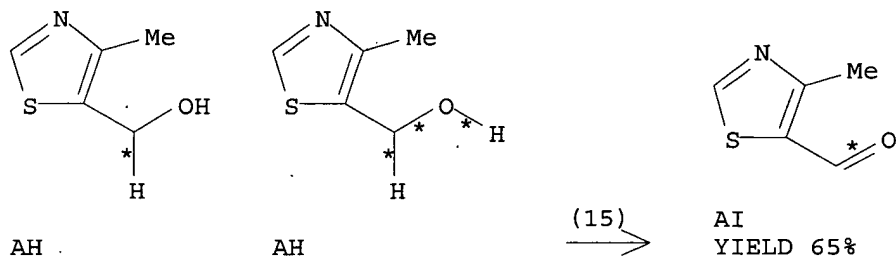
PRO AA 791854-32-5
NTE chemoselective

L3 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(15) OF 33 2 AH ==> AI + AJ

Updated Search

10509228



AJ
YIELD 11%

RX(15) RCT AH 1977-06-6

STAGE(1)

RGT C 3225-26-1 Piperidinooxy deriv., D 7631-86-9
SiO2
SOL 67-64-1 Me2CO
CON 10 minutes, room temperature

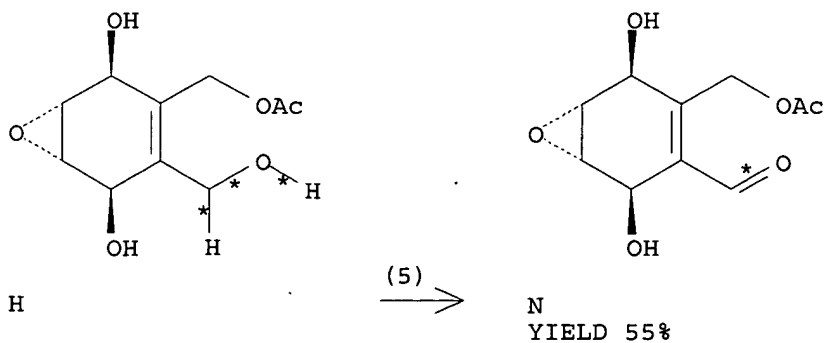
STAGE(2)

RGT E 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, 0 deg C

PRO AI 82294-70-0, AJ 20485-41-0

L3 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 87 ...H ==> N...



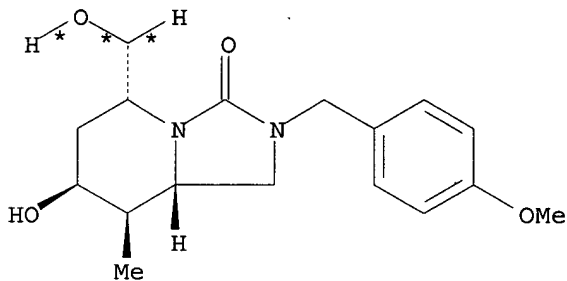
Updated Search

10509228

RX(5) RCT H 735317-25-6
RGT O 2564-83-2 Me4-piperidoxyl, P 7782-44-7 O2, Q
7758-89-6 CuCl
PRO N 735317-27-8
SOL 68-12-2 DMF

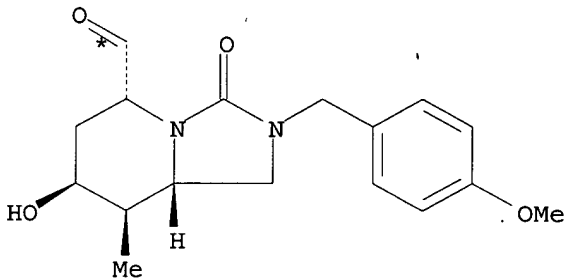
L3 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 120 ...V ==> H...



V

(6) >



H
YIELD 75%

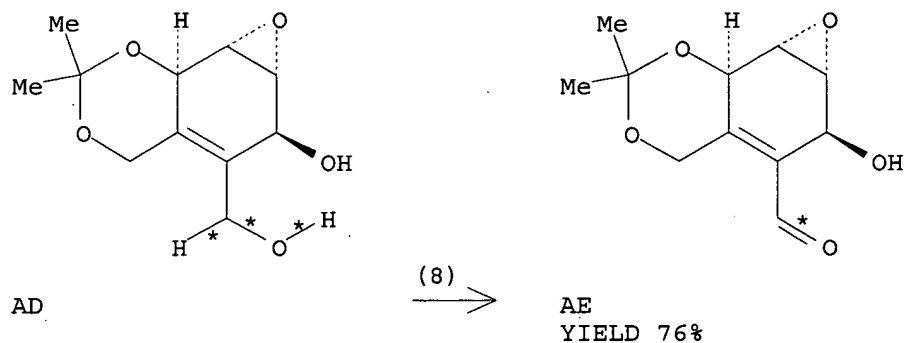
RX(6) RCT V 732278-69-2
RGT W 3240-34-4 PhI(OAc)2, X 2564-83-2 Me4-piperidoxyl, Y
75-75-2 MeSO3H
PRO H 732278-68-1
SOL 865-49-6 CDCl3
CON 3 hours, room temperature

L3 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(8) OF 307 ...AD ==> AE...

Updated Search

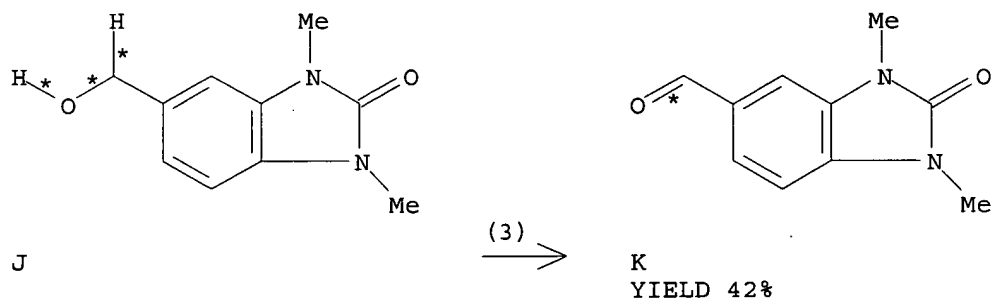
10509228



RX(8) RCT AD 701921-79-1
RGT AF 7782-44-7 O₂, AG 7758-89-6 CuCl, AH 2564-83-2
Me4-piperidoxyl
PRO AE 701921-80-4
SOL 68-12-2 DMF

L3 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 443 ...J ==> K...

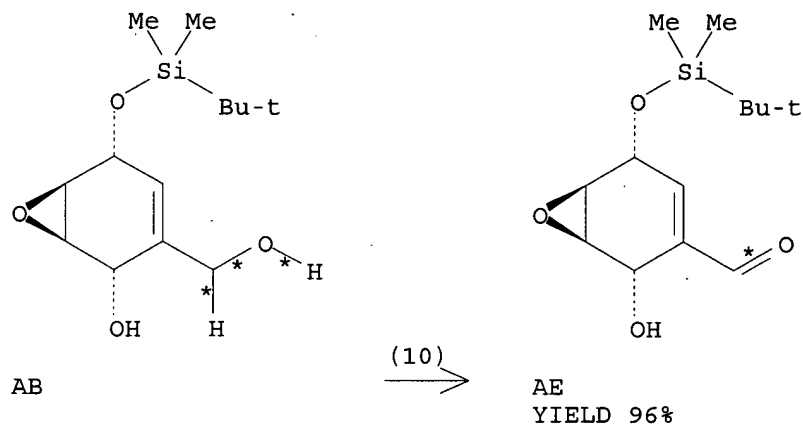


RX(3) RCT J 345657-96-7
RGT L 2564-83-2 Me4-piperidoxyl, M 128-09-6
Chlorosuccinimide
PRO K 55241-49-1
CAT 1112-67-0 Bu₄NCl
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 5.5 hours, room temperature, pH 8.6
NTE buffered soln.

L3 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(10) OF 115 ...AB ==> AE...

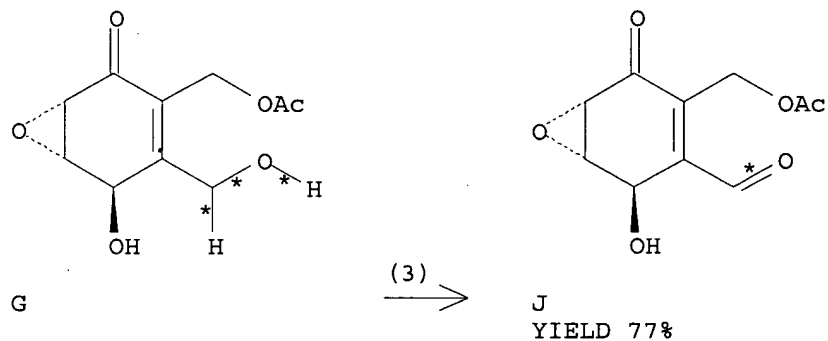
10509228



RX(10) RCT AB 678197-28-9
RGT AF 2564-83-2 Me4-piperidoxyl, AG 7782-44-7 O2, AH 7758-89-6 CuCl
PRO AE 678197-29-0
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

L3 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 100 ...G ==> J...



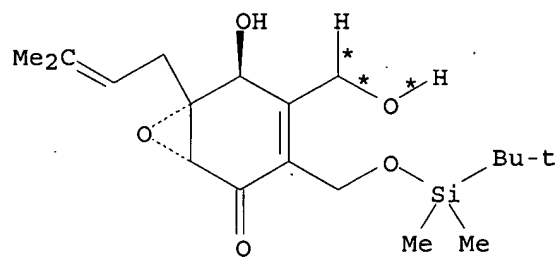
RX(3) RCT G 676263-76-6
RGT K 2564-83-2 Me4-piperidoxyl, L 7782-44-7 O2
PRO J 676263-78-8
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON room temperature
NTE chemoselective

L3 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 201 ...AF ==> AH...

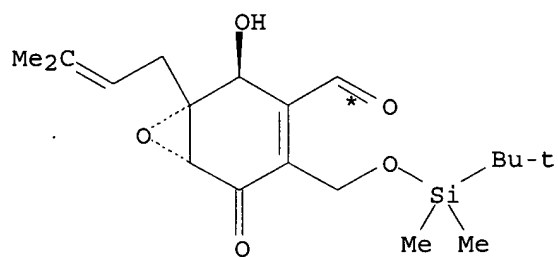
Updated Search

10509228



AF

(11) →



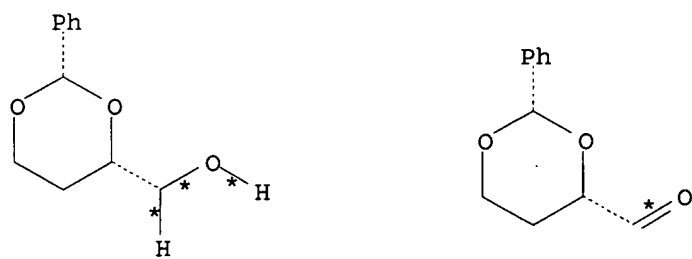
AH

YIELD 90%

RX(11) RCT AF 674358-50-0
RGT AI 2564-83-2 Me4-piperidoxyl, AJ 7782-44-7 O2
PRO AH 674358-53-3
CAT 7758-89-6 CuCl
SOL 68-12-2 DMF
CON 3 hours, room temperature
NTE chemoselective

L3 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 288 ...M ==> N...



M

(3) →

N
YIELD 70%

RX(3) RCT M 103773-79-1

Updated Search

10509228

STAGE(1)

RGT O 3240-34-4 PhI(OAc)₂, P 14691-89-5
1-Piperidinyloxy, 4-(acetylamino)-2,2,6,6-tetramethyl-
SOL 75-09-2 CH₂Cl₂
CON 14 hours, 18 deg C

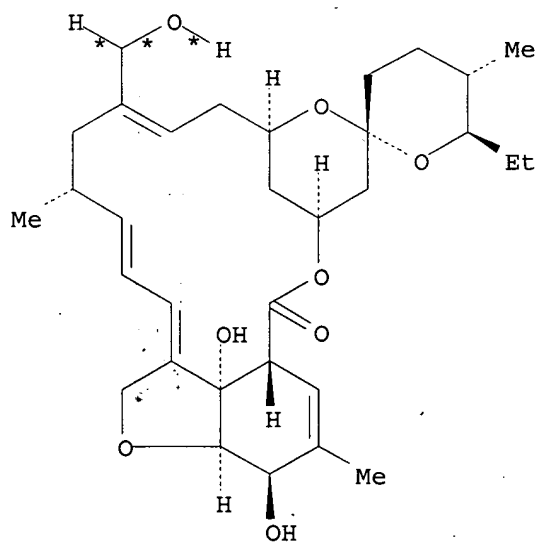
STAGE(2)

RGT E 144-55-8 NaHCO₃
SOL 7732-18-5 Water
CON 18 deg C

PRO N 145958-02-7

L3 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

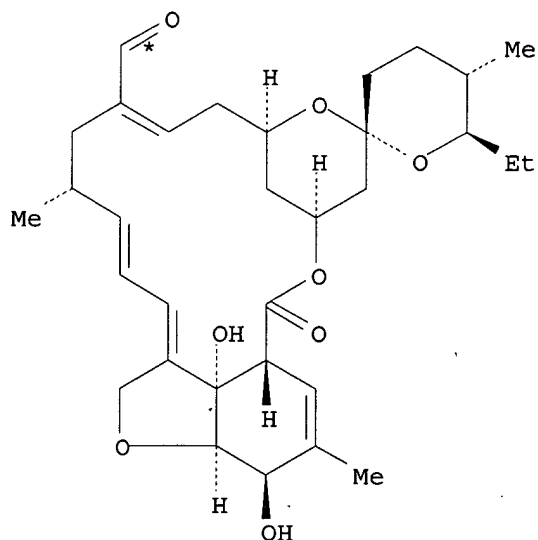
RX(5) OF 28 ...K ==> M...



K

(5) →

10509228

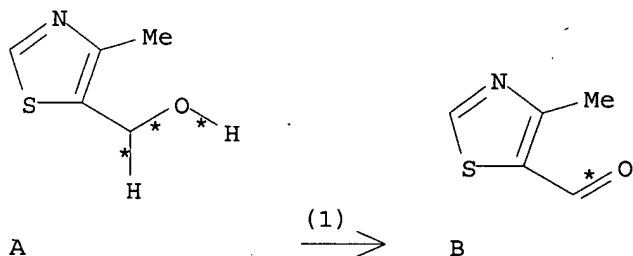


M
YIELD 87%

RX(5) RCT K 112774-81-9
RGT N 144-55-8 NaHCO₃, O 584-08-7 K₂CO₃, P 2564-83-2
Me₄-piperidoxyl, Q 1112-67-0 Bu₄NCl, R 128-09-6
Chlorosuccinimide
PRO M 112774-92-2
SOL 7732-18-5 Water, 75-09-2 CH₂Cl₂
CON 1 hour, room temperature
NTE regioselective

L3 ANSWER 23 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 5 ...A ==> B



RX(1) RCT A 1977-06-6
STAGE(1)
SOL 75-09-2 CH₂Cl₂
CON 5 minutes, room temperature
STAGE(2)
RGT C 144-55-8 NaHCO₃

Updated Search

10509228

SOL 7732-18-5 Water
CON SUBSTAGE(1) 30 - 32 deg C
SUBSTAGE(2) 5 - 10 minutes, 30 - 32 deg C

STAGE (3)

RGT D 7758-02-3 KBr, E 2564-83-2 Me4-piperidoxyl, F
7681-52-9 NaOCl

SOL 7732-18-5 Water

CON SUBSTAGE(1) 32 deg C -> 0 deg C

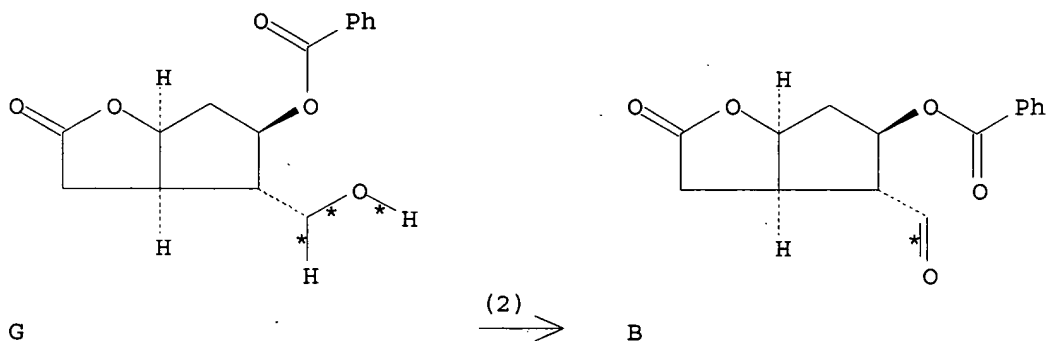
SUBSTAGE (3) 1 hour, 0 - 2 deg C

SUBSTAGE (4) 0 - 2 deg C

PRO B 82294-70-0

L3 ANSWER 24 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

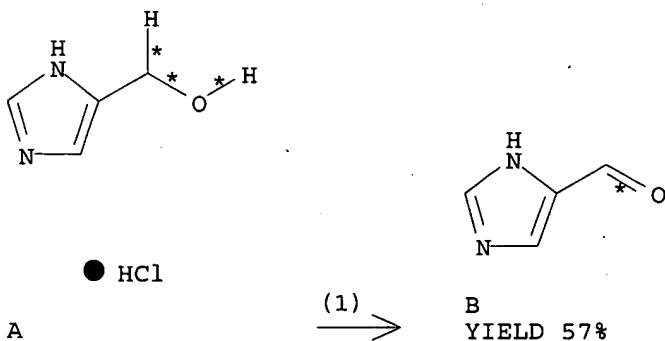
RX (2) OF 66 G ==> B...



RX(2) RCT G 39746-00-4
RGT H 7681-52-9 NaOCl, I 2564-83-2 Me4-piperidoxyl, J
7758-02-3 KBr
PRO B 39746-01-5
SOL 75-09-2 CH2Cl2

L3 ANSWER 25 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX (1) OF 3 A ==> B



Updated Search

10509228

RX(1) RCT A 32673-41-9

STAGE(1)

RGT C 2226-96-2 1-Piperidinyloxy,
4-hydroxy-2,2,6,6-tetramethyl-
SOL 75-09-2 CH₂Cl₂

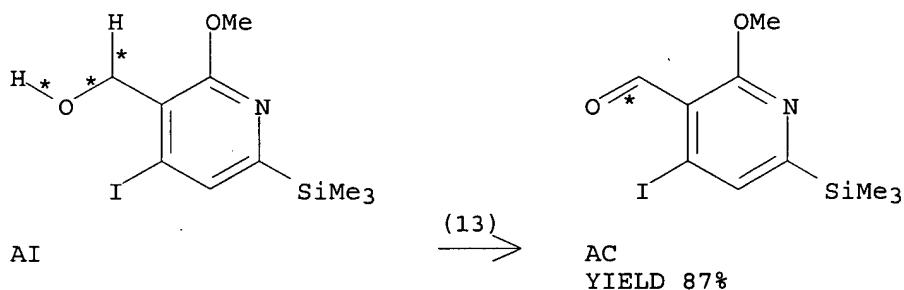
STAGE(2)

RGT D 7681-52-9 NaOCl
SOL 7732-18-5 Water

PRO B 3034-50-2

L3 ANSWER 26 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(13) OF 249 AI ==> AC

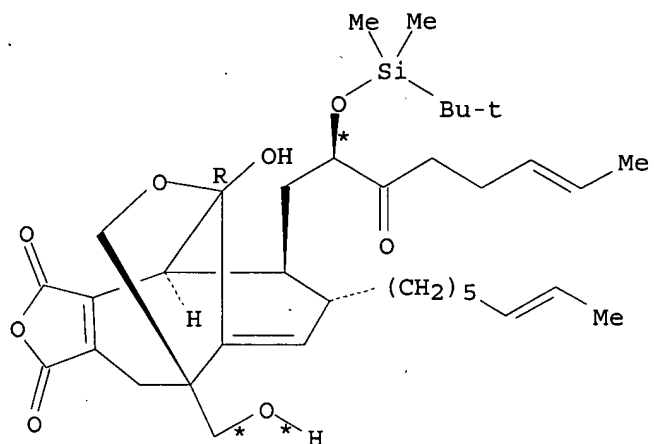


RX(13) RCT AI 375346-05-7
RGT AO 7681-52-9 NaOCl, AP 2564-83-2 Me4-piperidoxyl
PRO AC 174092-75-2
SOL 7732-18-5 Water, 108-88-3 PhMe
NTE oxidn. at 0-5° for 2 h

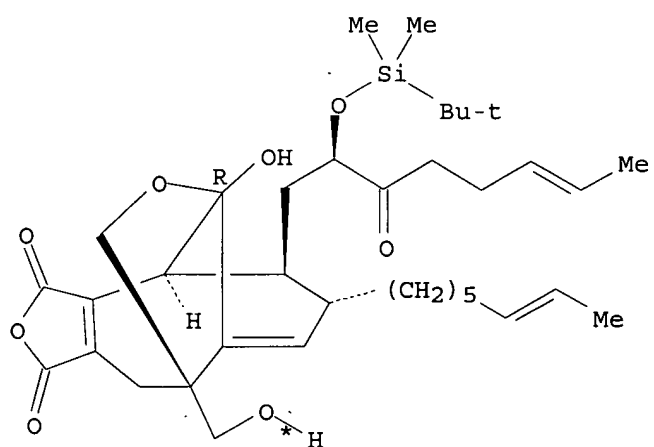
L3 ANSWER 27 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(362) OF 443 COMPOSED OF RX(38), RX(39), RX(40), RX(1), RX(43)
RX(362) 2 I + 2 BX + BA ==> DI

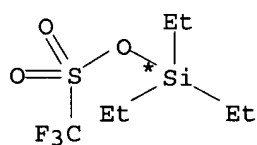
10509228



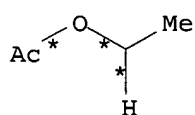
I



I



2 BX

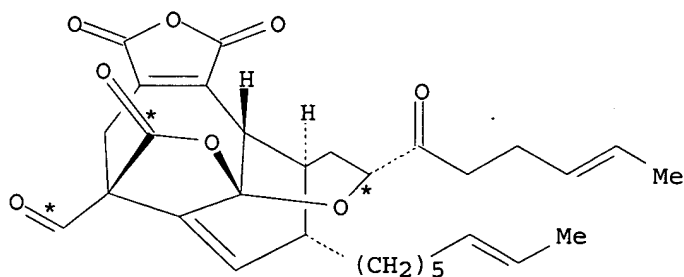


BA

5
STEPS
→

Updated Search

10509228



DI
YIELD 95%

RX(38) RCT I 241819-26-1, BX 79271-56-0

STAGE(1)

RGT O 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT F 7732-18-5 Water

PRO DB 241819-27-2

RX(39) RCT DB 241819-27-2

STAGE(1)

RGT BS 87413-09-0 Martin's reagent
SOL 7732-18-5 Water, 71-43-2 Benzene

STAGE(2)

RCT BA 141-78-6
RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO DC 242142-83-2, DD 412943-13-6

RX(40) RCT DC 242142-83-2

STAGE(1)

RGT CV 2564-83-2 Me4-piperidoxyl, DE 3240-34-4
PhI(OAc)2
SOL 75-05-8 MeCN

STAGE(2)

RGT P 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO A 241819-29-4

RX(1) RCT A 241819-29-4

STAGE(1)

RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

Updated Search

10509228

STAGE(2)

RGT D 75-75-2 MeSO₃H

SOL 67-66-3 CHCl₃

PRO B 241819-30-7

RX(43) RCT B 241819-30-7

STAGE(1)

RGT P 144-55-8 NaHCO₃

SOL 75-09-2 CH₂Cl₂

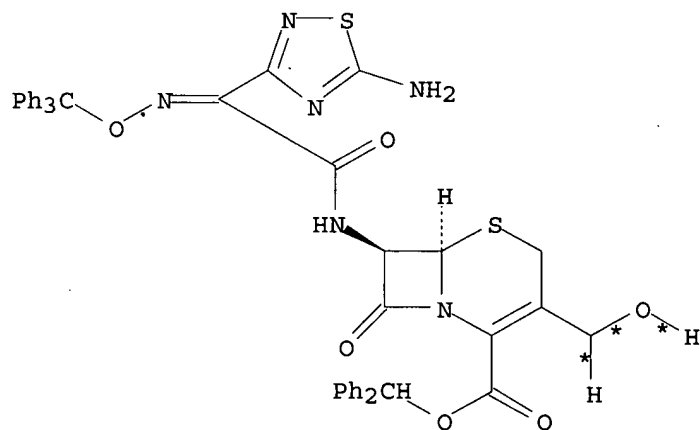
STAGE(2)

RGT BS 87413-09-0 Martin's reagent

PRO DI 241819-31-8

L3 ANSWER 28 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

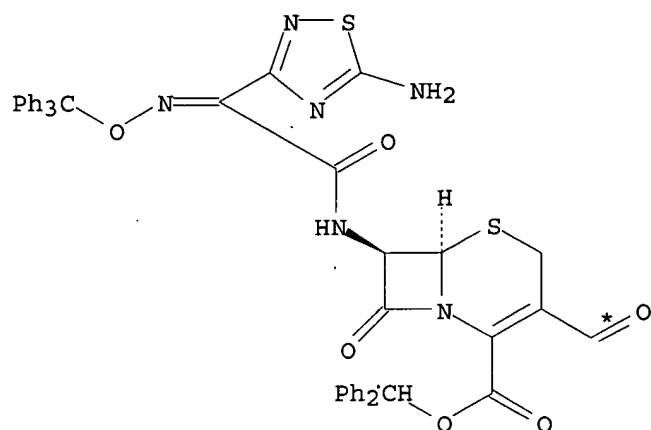
RX(2) OF 29 ...D ==> G...



D

(2) →

10509228



G

RX(2) RCT D 376653-36-0

STAGE(1)

RGT H 7758-02-3 KBr, I 144-55-8 NaHCO3, J 2564-83-2
Me4-piperidoxyl
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

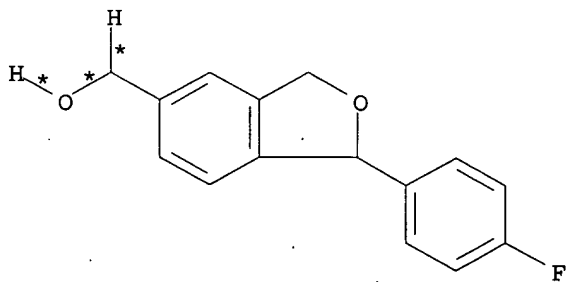
STAGE(2)

RGT K 7681-52-9 NaOCl
SOL 7732-18-5 Water

PRO G 376653-37-1
NTE alternative prepn. shown

L3 ANSWER 29 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 28 ...U ==> Z...

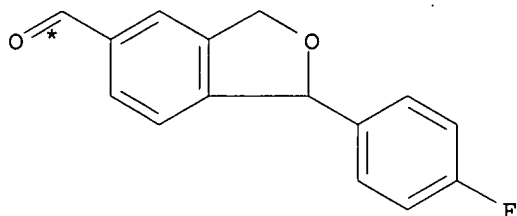


U

(6) →

Updated Search

10509228



Z
YIELD 84%

RX(6) RCT U 335612-71-0

STAGE(1)

RGT AA 144-55-8 NaHCO₃, AB 1643-19-2 Bu₄N.Br, AC
2564-83-2 Me₄-piperidoxyl
SOL 141-78-6 AcOEt

STAGE(2)

RGT AD 7681-52-9 NaOCl
SOL 7732-18-5 Water

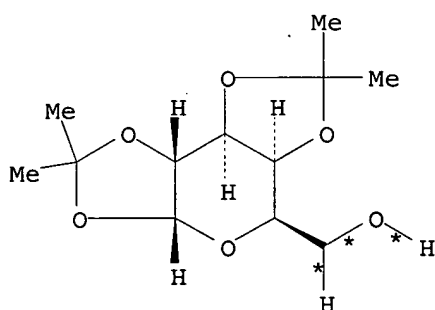
STAGE(3)

SOL 7732-18-5 Water

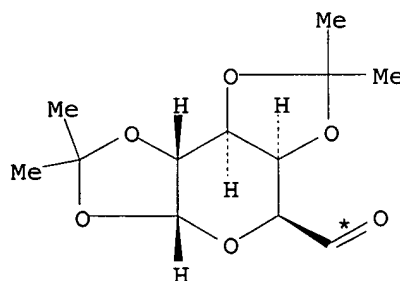
PRO Z 335612-72-1

L3 ANSWER 30 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(11) OF 18 AC ==> AD



AC



AD
YIELD 97%

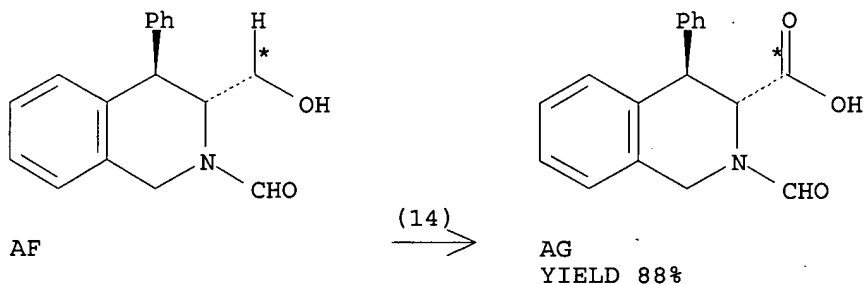
RX(11) RCT AC 4064-06-6
RGT D 74-89-5D MeNH₂, J 2564-83-2 Me₄-piperidoxyl
PRO AD 4933-77-1
SOL 75-09-2 CH₂Cl₂
NTE STEREOSELECTIVE

L3 ANSWER 31 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

Updated Search

10509228

RX(14) OF 52 ...AF ==> AG...



RX(14) RCT AF 294869-50-4

STAGE(1)

RGT AH 2564-83-2 Me4-piperidoxyl, AI 144-55-8 NaHCO₃,

AJ 7758-02-3 KBr, AK 1112-67-0 Bu₄NCl

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT AL 7681-52-9 NaOCl, AI 144-55-8 NaHCO₃, AM 7647-14-5 NaCl

SOL 7732-18-5 Water

STAGE(3)

RGT Q 1310-73-2 NaOH

STAGE(4)

RGT P 7647-01-0 HCl

STAGE(5)

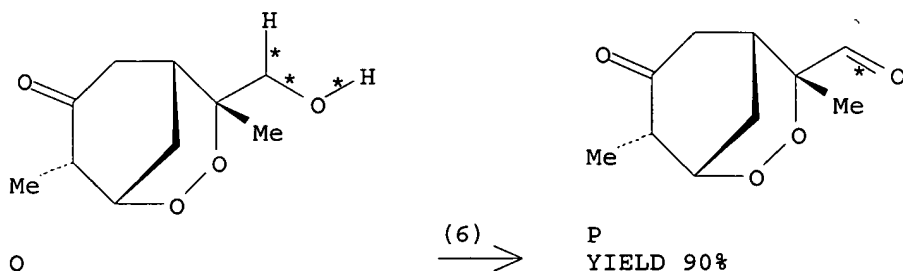
SOL 75-09-2 CH₂Cl₂

PRO AG 294869-51-5

NTE STEREOSELECTIVE

L3 ANSWER 32 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(6) OF 7 O ==> P



RX(6) RCT O 160420-93-9

RGT C 87-90-1 Isocyanuric chloride, D 2564-83-2

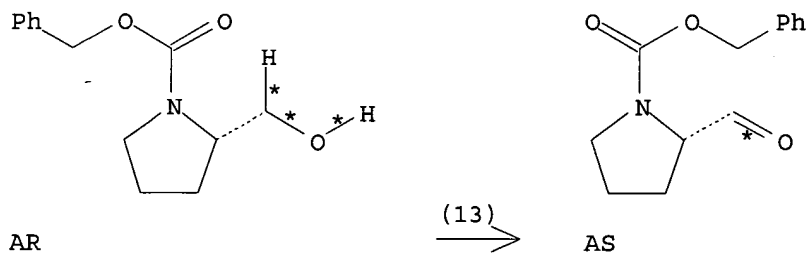
Updated Search

10509228

Me4-piperidoxyl, E 127-09-3 AcONa
PRO P 160497-32-5
SOL 75-09-2 CH2Cl2

L3 ANSWER 33 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(13) OF 84 ...AR ==> AS...



RX(13) RCT AR 6216-63-3

STAGE(1)

RGT AT 7647-15-6 NaBr

SOL 7732-18-5 Water, 108-88-3 PhMe

STAGE(2)

RGT AU 2564-83-2 Me4-piperidoxyl

STAGE(3)

RGT G 497-19-8 Na2CO3, AV 7681-52-9 NaOCl

SOL 7732-18-5 Water

PRO AS 71461-30-8

L3 ANSWER 34 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

RX(3) OF 4 I ==> J

<-----User Break----->

=> d his

(FILE 'HOME' ENTERED AT 19:49:32 ON 12 OCT 2006)

FILE 'CASREACT' ENTERED AT 19:49:46 ON 12 OCT 2006

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 38 S L1 FULL

L4 0 S L3 AND SHIOMI, Y?/AU

L5 0 S L3 AND UNO, O?/AU

L6 0 S L3 AND OHTA, A?/AU

L7 0 S L3 AND SUNAKAMI, T?/AU

FILE 'REGISTRY' ENTERED AT 19:58:36 ON 12 OCT 2006

L8 1 S 7782-44-7/RN

SET NOTICE 1 DISPLAY

Updated Search

10509228

SET NOTICE LOGIN DISPLAY

FILE 'CASREACT' ENTERED AT 20:01:06 ON 12 OCT 2006

=> d l3, ibib abs fhlt, 1-38

COMMAND INTERRUPTED

REENTER FILE 'CASREACT'

AND TRY AGAIN, OR ENTER '?' FOR MORE INFORMATION.

Your command did not complete due to a temporary system problem. To recover, reenter the file you are in now. Then, any command that is normally available to you may be used. No cost summary for the current file will be displayed. After reentering the current file you may retry your command. Also, you may wish to SAVE your search query. This can be done in any file. If you cannot access your current file, or if your command fails a second time, notify the Help Desk. Enter "HELP STN" for information on contacting the nearest STN Help Desk by telephone or by using the SEND command in STNMAIL file.

=> d l3, ibib fhlt, all

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> d l3, ibib abs fhlt

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	919	((549/70) or (546/315)).CCLS.	US-PGPUB; USPAT	OR	OFF	2006/10/12 22:28
L2	92	1 and heterocyclic and aldehyde	USPAT	OR	OFF	2006/10/12 22:30
L3	123	1 and heterocyclic and aldehyde	US-PGPUB; USPAT	OR	OFF	2006/10/12 22:30